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#### **Abstract**

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

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# **1 Introduction**

 Quantum computing is an emerging paradigm of computation where quantum physical phenomena, such as entanglement and superposition, are used to obtain an advantage over classical computation. A testament to the richness of the field is the variety of computational models: quantum Turing machines [\[3\]](#page-15-0), quantum circuits [\[18,](#page-15-1) [16\]](#page-15-2), measurement-based quantum computation [\[4,](#page-15-3) [6\]](#page-15-4), linear optical circuits [\[13\]](#page-15-5), among others. Some of these models have been shown to be equivalent in terms of computational power and complexity. For instance, Yao's equivalency result [\[18\]](#page-15-1) shows that polynomial-time quantum Turing machine are computationally equivalent to uniform and poly-size quantum circuit families.

<sup>24</sup> A lot of effort has been put on developing high-level quantum programming languages to allow programmers to abstract themselves from the technicalities of these low-level models. Towards that end, several verification techniques such as type systems [\[9\]](#page-15-6) or categorical approaches for reasoning on programs semantics [\[2,](#page-15-7) [11\]](#page-15-8) have been studied and developed to ensure the physical reality of compiled programs, for example, by ensuring that it preserves the main properties of quantum mechanics such as no-cloning theorem [\[1\]](#page-15-9) or unitarity [\[8\]](#page-15-10). <sup>30</sup> An important line of research in this area involves checking polytime termination of quantum programs [\[5,](#page-15-11) [17,](#page-15-12) [10\]](#page-15-13).

 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

<span id="page-0-0"></span>

**Figure 1** Classical vs. quantum branching.

 between the two branches (Figure [1\)](#page-0-0). However, this is not necessarily the case in the quantum setting, as a consequence of no-cloning: in a quantum circuit, the two branches may

Mário Silva will present this work if selected.

 contain operations on the same qubits, and thus require an implementation in series. This results in a circuit whose total depth is the sum of the depths of the two branches as illustrated by Figure [1.](#page-0-0) In [\[19\]](#page-15-14), while trying to encode efficient operations over quantum data structures, the authors encounter this problem which they have coined *branch sequentialization*. While the authors provide a heuristic for avoiding branch sequentialization, it is only applicable <sup>49</sup> in a few precise examples. Given the importance of preserving the time complexity of a program in its circuit implementation, there is an interest in discovering general techniques that avoid the problem of branch sequentialization altogether.

 *Motivating Example.* Consider the program PAIRS defined in Figure [2.](#page-1-0) The procedure 53 pairs takes as input a sorted set  $\bar{q}$  of qubits (i.e., a collection of pairwise distinct qubits) on which it will perform operations. By language design, pairs immediately terminates  $\frac{1}{55}$  whenever  $\overline{q}$  is empty. First, pairs checks that the number of qubits in  $\overline{q}$ , given by its size  $|\overline{q}|$ , is larger than 1 to enter the recursive case, otherwise it applies a NOT gate to the remaining qubit (line 9). On line 3, the program will branch depending on the state  $\bar{q}[1,2]$  of the first two qubits in  $\bar{q}$ . Out of all four cases (lines 4-7), pairs only performs an operation when the first two qubits are in state  $|00\rangle$  or  $|11\rangle$ , in which case it performs a recursive call on  $\bar{q} \ominus [1, 2]$ ,  $\frac{60}{100}$  the sorted set  $\bar{q}$  where the first and second qubits have been removed.

61 With  $x \in \{0, 1\}^*$  and  $y \in \{0, 1\}$ , given the input state ∣*xy*⟩, pairs will apply a *NOT* gate to *y* if and only if *x* is a string consisting only of sequences of 00 and 11. Put another way, pairs encodes a unitary transformation that inverts the state of the last qubit of an  $\epsilon_7$  input when *x* belongs to the regular language 68 defined by  $(00 \, | \, 11)^*$ .

 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.

Let us now turn to finding a circuit im-

<span id="page-1-0"></span>

#### **Figure 2** Branching program PAIRS.

 plementation for the recursive case of pairs. Consider the two compilation strategies **(a)** and **(b)** shown in Figure [3.](#page-2-0) While Strategy **(a)** could be considered the more direct approach to building the circuit, at each recursive call the size of the circuit for pairs is the sum of  $\pi$  the sizes of each branch. On the other hand, while the strategy in **(b)** requires the creation of an ancilla and the use of extra Toffoli gates, it only requires the implementation of one call <sup>79</sup> to pairs. As a consequence, the strategies (a) and (b) result in circuits of depth  $\Theta(|\bar{q}|2^{|\bar{q}|})$ <sup>80</sup> and  $\Theta(|\bar{q}|)$ , respectively, showing how implementing the branches sequentially can result in an exponential blowup in circuit size. It is simple enough to find a compilation strategy that <sup>82</sup> prevents the duplication of pairs in the recursive case. However, this becomes much less trivial once we consider programs with more complex recursive calls.

<sup>84</sup> *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\)](#page-7-0). 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 [\[10\]](#page-15-13) whose expressive power is illustrated through many

<span id="page-2-0"></span>

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

<sup>92</sup> examples (see Table [1\)](#page-13-0);

<sup>93</sup> ► We introduce a compilation strategy **compile**<sup>+</sup> from PFOQ to quantum circuits based on two subroutines **compr**<sup>+</sup> (Algorithm [1\)](#page-8-0) and **optimize**<sup>+</sup> (Algorithm [2\)](#page-9-0): while **compr**<sup>+</sup> 94 <sup>95</sup> just generates the compiled circuit by a simple structural induction on program statements, <sup>96</sup> **optimize**<sup>+</sup> perform some optimization by merging (recursive) procedure calls in different <sup>97</sup> branches in the program.

 $\mathcal{P}_{98}$  We show that the **compile**<sup>+</sup> is sound, i.e., the generated circuit fairly simulates the input <sup>99</sup> program: this correctness result lies on the orthogonality of the control structures used <sup>100</sup> in the **optimize**<sup>+</sup> subroutine (Lemma [11\)](#page-10-0).

 $101 \equiv$  On PFOQ programs, we exhibit a direct improvement on size complexity of the generated <sup>102</sup> circuit with respect to the compilation algorithm studied in [\[10\]](#page-15-13) (Theorem [12\)](#page-11-0).

<sup>103</sup> We show that, on BFOQ programs, **compile**<sup>+</sup> produces circuits whose size is asymptotically bounded by their level (Theorem [13\)](#page-12-0), 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 [\[15,](#page-15-15) [14\]](#page-15-16) (or at least its number of non-Clifford gates  $[12, 7]$  $[12, 7]$ , with techniques such as gate substitution, graph-rewriting, among others.

 Resource optimization for high-level quantum programs is still a relatively undeveloped research area as it involves the asymptotic consideration of families of circuits. Such an issue has strong connections with programming language-based characterizations of quantum polynomial time classes [\[17,](#page-15-12) [5,](#page-15-11) [10\]](#page-15-13) as, by design, their set of programs is sound and complete for uniform families of quantum circuits of polynomial size, as per Yao's equivalency theorem. While [\[17,](#page-15-12) [5\]](#page-15-11) provide non-constructive proofs of the existence of quantum circuits of polynomial size, [\[10\]](#page-15-13) introduces a programming language that avoids an exponential blowup in the complexity of recursive (quantum) branching with a direct compilation strategy for ensuring polysized circuit representations. However this strategy still performs branch sequentialization and generates polynomial bounds whose degree is not accurate.

<span id="page-3-0"></span> $(P_{\text{rograms}})$   $P(\bar{q}) \triangleq D::S$ (Procedure declarations)  $D \triangleq \varepsilon | \text{ decl proc}[x](\bar{q}) \{S\}, D$  $(Statements)$   $S \triangleq \text{skip}; |\bar{q}[i] \ast = U^f(j); | S S | \text{if } b \text{ then } S \text{ else } S$  $|$ **qcase**  $\bar{q}$ [i] **of**  $\{0 \rightarrow S, 1 \rightarrow S\}$  **| call** proc[i](s);

**Figure 4** Syntax of FOQ programs.

# <span id="page-3-1"></span><sup>122</sup> **2 First-Order Quantum Programming Language**

<sup>123</sup> We consider the foq (First-Order Quantum) programming language with quantum control,  $124$  introduced in [\[10\]](#page-15-13) to characterize quantum polynomial time. A complete account of its <sup>125</sup> syntax and its semantics is given in Appendix [A.](#page-16-0)

# <sup>126</sup> **2.1 Syntax**

127 A FOQ program  $P \triangleq D$  ∷ S is defined in Figure [4](#page-3-0) by a list of procedure declarations D and a program statement S . The language include 4 basic datatypes for expressions. *Sorted set* expressions s are either variables  $\bar{q}$ , the empty sorted set nil, or  $s \in [i]$ , the sorted set s where the i-th element has been removed. Intuitively, a sorted set is a list of unique (i.e., non-duplicable) qubit pointers. *Integer* expressions, noted i*,*j, are either an integer variable x, a constant *n*, an addition by a constant i±*n* or the size of a sorted set ∣s∣. *Boolean* expressions b are defined in a standard way using boolean operators and arithmetic operators, e.g., i > j. Finally, *qubit* expressions are of the shape s[i] which denotes the i-th qubit pointed 135 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 <sup>136</sup> sugar on sorted state of pointing to the *n*-th *last* qubit in the set, by defining for any  $n \ge 1$ ,  $_{137}$   $\bar{q}[-n] \triangleq \bar{q}[[\bar{q}]-n+1].$ 

138 A procedure of name proc is defined by a procedure declaration **decl** proc[x] $(\bar{q})$ {S<sup>proc</sup>} 139 which takes a sorted set  $\bar{q}$  and an (optional) integer x as input parameters and executes the <sup>140</sup> *procedure statement* S<sup>proc</sup>. Let Procedures be an enumerable set of procedure names. We 141 will write S instead of S<sup>proc</sup> when the procedure is clear from context, and we denote by 142 proc  $∈$  P the fact that proc appears in D. Given two statements S, S', S  $∈$  S' denotes the fact that S is a substatement of S'. Furthermore, we have that proc  $\epsilon$  S holds if there are i and s 144 such that **call**  $\text{proc}[i](s)$ ;  $\in$  S.

<sup>145</sup> Statements include the no-op instruction, unitary operations, sequences, classical and <sup>146</sup> quantum conditionals, and procedures calls. Of these, we highlight the quantum condi- $_{147}$  tional **qcase**  $\bar{q}[i]$  of  $\{0 \rightarrow S_0, 1 \rightarrow S_1\}$ , which allows branching by executing statements  $S_0$ 148 and  $S_1$  in superposition according to the state of qubit  $\bar{q}[i]$ , and also the procedure call <sup>149</sup> **call** proc[i](s);, which runs procedure proc with *integer expression* i and *sorted set* expression <sup>150</sup> s, a list of unique qubit pointers. The quantum conditional can be extended to *n* qubits  $q \text{ case } \bar{q}[i_1, \ldots, i_n] \text{ of } \{0^n \to S_{0^n}, \ldots, 1^n \to S_{1^n}\}$  in a standard way as used in Figure [2.](#page-1-0)

In a statement  $\bar{q}[i] \equiv U^f(j)$ ; if the integer expression j evaluates to *n*, then the unitary operator  $\llbracket U^f \rrbracket(n)$  corresponding to the unary construct  $U^f(j)$  is applied to qubit  $\bar{q}[i]$ .<br>For approximative numbers these constructs are permeaterized by some pelmonial times <sup>154</sup> For expressivity purposes, these constructs are parameterized by some polynomial-time 155 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  $R_n \triangleq [\text{Ph}^{\lambda x. \pi/2^{x-1}}](n)$  with  $[\text{DH}^{\{1\}}(\alpha) \triangleq \ell^{1} \geq 0]$ . Other hesis weave gates are the *NOT* and the *P* gate (see [10])  $\llbracket \text{Ph}^f \rrbracket(n) \triangleq \left( \begin{smallmatrix} 1 & 0 \\ 0 & e^{if(n)} \end{smallmatrix} \right)$ <sup>157</sup> [Ph<sup>*I*</sup>]](*n*)  $\triangleq$  ( $\frac{1}{0}$   $\frac{0}{e^{i f(n)}}$ ). Other basic unary gates are the *NOT* and the *R<sub>Y</sub>* gate (see [\[10\]](#page-15-13)). <sup>158</sup> We also make use of some syntactic sugar to describe statements encoding constant-time

<sup>159</sup> quantum operations. For instance, the *CNOT*, *SW AP*, and Toffoli gates can be defined by:

 $\frac{160}{161}$  $CNOT(\bar{q}[i], \bar{q}[j]) \triangleq$  **qcase**  $\bar{q}[i]$  **of**  $\{0 \rightarrow \text{skip}; 1 \rightarrow \bar{q}[j] \rightarrow \text{NOT}\}$ 

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

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

<sup>165</sup> We define notions of rank that provide quantitative information on the recursion level of <sup>166</sup> a given program or procedure.

<sup>167</sup> ▶ **Definition 1** (Rank)**.** *Given a* foq *program* P*, the rank of a procedure* proc *in* P*, denoted* <sup>168</sup> *rk*P(proc)*, is defined as follows:*

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

<sup>170</sup> where  $\max(\emptyset) \triangleq 0$ . The rank of a program *is defined as the maximum rank among all* 171 *procedures, i.e., for a program*  $P \triangleq D :: S$ *, we have that*  $rk(P) \triangleq \max_{\text{proc}\in D} rk_P(\text{proc})$ *.* 

<sup>172</sup> ▶ **Example 2.** The program PAIRS given in Figure [2](#page-1-0) has rank 1, since *rk*(PAIRS) ≜ 173 max $_{\text{proc}\in\text{PAIRS}}$   $rk_{\text{P}}(\text{proc}) = rk(\text{pairs}) = 1$ .

# <sup>174</sup> **2.2 Semantics**

<sup>175</sup> 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 <sup>176</sup> 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 178 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 179 pointers into consideration when evaluating e. For example, we have that  $(\bar{q}[2], [1, 4, 5]) \parallel_{\mathbb{N}}$ 180 4 (the second qubit is of index 4),  $(\bar{q}[4], [1, 4, 5]) \Downarrow N$  0 (index 0 is used for error), and  $\bar{q}$  ( $\bar{q}$   $\ominus$  [3], [1, 4, 5])  $\downarrow$ <sub>*C*(N)</sub> [1, 4] (the third qubit has been removed).

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

The big-step semantics  $\cdot \longrightarrow \cdot$  is defined as a relation in  $\bigcup_{n\in\mathbb{N}} \text{Conf}_n \times \mathbb{N} \times \text{Conf}_n$ . When  $c \stackrel{m}{\longrightarrow} c'$  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 level<sub>P</sub> $(n)$ , is defined by

$$
level_P(n) \triangleq \max\{m \in \mathbb{N} \mid \exists |\phi\rangle, |\phi'\rangle \in \mathcal{H}_{2^n}, (S, |\phi\rangle, \mathcal{S}_n, l_n) \stackrel{m}{\longrightarrow} (\top, |\phi'\rangle, \mathcal{S}_n, l_n)\},
$$

190 with  $S_n \triangleq \{1, \ldots, n\}$  and  $l_n \triangleq [1, \ldots, n]$ .

 ▶ **Example 3.** Consider the program PAIRS of Figure [2.](#page-1-0) We have that each procedure call removes two qubits until it reaches a case of input size ∣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,  $\text{level}_{\text{PAIRS}}(n) = \lfloor \frac{n}{2} \rfloor + 1 = O(n)$ .

# <sup>195</sup> **2.3 Polytime fragments of FOQ**

 In [\[10\]](#page-15-13), 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  $\rightarrow_P \subseteq$  Procedures  $\times$  $_{201}$  Procedures is defined for any two procedures  $\text{proc}_1$ ,  $\text{proc}_2 \in S$  as  $\text{proc}_1 \rightarrow_{P} \text{proc}_2$  whenever <sub>202</sub> proc<sub>2</sub> ∈ S<sup>proc<sub>1</sub>. The partial order ≥<sub>P</sub> is then the transitive closure of  $\rightarrow$ <sub>P</sub>, and  $\sim$ <sub>P</sub> denotes the</sup> equivalence relation where  $\text{proc}_1 \sim_P \text{proc}_2$  if  $\text{proc}_1 \geq_P \text{proc}_2$  and  $\text{proc}_2 \geq_P \text{proc}_1$  both hold. <sup>204</sup> call proc' ∈ S<sup>proc</sup> is a *recursive* procedure call whenever proc ~<sub>P</sub> proc'. The strict order ><sub>P</sub> 205 is defined as  $\text{proc}_1 \succ_{\text{P}} \text{proc}_2$  if  $\text{proc}_1 \succeq_{\text{P}} \text{proc}_2$  and  $\text{proc}_1 \not\downarrow_{\text{P}} \text{proc}_2$  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 209 programs, we use the notion of *width of a procedure* proc in a program P, noted width<sub>P</sub>(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.

212 **► Definition 4** (Width of a procedure). *Given*  $P \in F \circ Q$  *and* proc  $\in P$ *, the* width of proc in P,  $p_{\text{213}}$  noted width<sub>P</sub>(proc)*, is defined as* width<sub>P</sub>(proc)  $\triangleq w_{\text{P}}^{\text{proc}}(\text{S}^{\text{proc}})$ *, where*  $w_{\text{P}}^{\text{proc}}(\text{S})$  *is the* width <sup>214</sup> of the procedure proc in P relative to statement S*, defined inductively as:*

215 
$$
w_{\text{P}}^{\text{proc}}(\text{skip};) = w_{\text{P}}^{\text{proc}}(q \ast = U^{f}(i);) \triangleq 0,
$$
216 
$$
w_{\text{P}}^{\text{proc}}(S_{1} S_{2}) \triangleq w_{\text{P}}^{\text{proc}}(S_{1}) + w_{\text{P}}^{\text{proc}}(S_{2}),
$$
217 
$$
w_{\text{P}}^{\text{proc}}(\text{if } b \text{ then } S_{\text{true}} \text{ else } S_{\text{false}}) \triangleq \max(w_{\text{P}}^{\text{proc}}(S_{\text{true}}), w_{\text{P}}^{\text{proc}}(S_{\text{false}})),
$$
218 
$$
w_{\text{P}}^{\text{proc}}(\text{qcase } q \text{ of } \{0 \rightarrow S_{0}, 1 \rightarrow S_{1}\}) \triangleq \max(w_{\text{P}}^{\text{proc}}(S_{0}), w_{\text{P}}^{\text{proc}}(S_{1})),
$$
219 
$$
w_{\text{P}}^{\text{proc}}(\text{call } \text{proc}'[i](s);) \triangleq \begin{cases} 1 & \text{if } \text{proc } \sim_{\text{P}} \text{proc}',\\ 0 & \text{otherwise}. \end{cases}
$$

221 Let WIDTH<sub>51</sub> be the set of programs with procedures of width at most 1. Finally, define 222 PFOQ ≜ FOQ∩WF∩WIDTH<sub>≤1</sub>. We will show that PFOQ can be restricted to a fragment, denoted <sup>223</sup> bfoq (for Basic foq), that is still complete for polynomial time and where the compilation <sup>224</sup> procedure conserves the intuitive complexity of the program. Let basic denote the set of <sup>225</sup> programs where i) procedures do not use classical inputs ii) procedure call parameters are z<sub>26</sub> restricted to sorted set variables  $\bar{q}$  or to a fixed sorted set s (s is fixed for each BFOQ program). 227 Then, we define BFOQ  $\triangleq$  BASIC ∩ PFOQ. It trivially holds that BFOQ  $\subseteq$  PFOQ  $\subseteq$  FOQ.

<span id="page-5-0"></span>▶ **Example 5** (Quantum Full Adder ∈ 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  $(a + b + c_{\text{in}})$ .

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

<sup>228</sup> where *c*in and *c*out encode the *carry-in* and *carry-out* values, respectively. The operator

*ADD* corresponds to the circuit in Figure [6](#page-7-1) and is described by the program FA below.



241 It holds that FA ∈ FOQ ∩ WF and that width<sub>FA</sub>(fullAdder) = 1. Therefore, FA ∈ PFOQ. Also, FA is clearly in bfoq as there is only one recursive call and no integer parameter.

<span id="page-6-0"></span> ▶ **Example 6** (Quantum Fourier Transform ∈ bfoq)**.** The quantum Fourier transform can be described by the program QFT below



 The program consists of three procedures, qft, shift, and rot, and is in pfoq since it is 258 in WF and width $_{\text{QFT}}(\text{gtt}) = \text{width}_{\text{QFT}}(\text{shift}) = \text{width}_{\text{QFT}}(\text{rot}) = 1$ . All procedure calls are 259 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](#page-7-2) 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.

<span id="page-6-2"></span> $\mathcal{P}_{268}$   $\blacktriangleright$  Lemma 7 (Polynomial level [\[10\]](#page-15-13)). *For any PFOQ program* P, level $_{\mathrm{P}}(n)$  =  $O(n^{rk(\mathrm{P})})$ .

 The set pfoq of programs was shown to be sound and complete for the class fbqp, of function computable in quantum polynomial time [\[10\]](#page-15-13).

<span id="page-6-1"></span> ▶ **Theorem 8** (pfoq-Soundness and Completeness [\[10\]](#page-15-13))**.** *For every function f in* fbqp*, there*  $\frac{1}{272}$  *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*  $\overrightarrow{PROQ}$  *, if* P *computes*  $f: \{0,1\}^* \rightarrow \{0,1\}^*$ , *with probability*  $p \in \left(\frac{1}{2}, 1\right]$  *then*  $f \in FBQP$ *.* 

<span id="page-7-2"></span>

**Figure 5** Circuit for the QFT as defined by the program in Example [6.](#page-6-0)

<span id="page-7-1"></span>

**Figure 6** Quantum Full Adder circuit (Example [5\)](#page-5-0) for input size 10.

- <span id="page-7-0"></span><sup>275</sup> Being a strict subset of pfoq, bfoq is trivially sound. Surprisingly, it is also complete.
- <sup>276</sup> ▶ **Theorem 9** (bfoq-Soundness and Completeness)**.** *Theorem [8](#page-6-1) holds for* bfoq*.*

<sup>277</sup> **Proof.** Soundness is trivial since bfoq is contained in pfoq, and completeness is given <sup>278</sup> analogously to the proof of [\[10,](#page-15-13) Theorem 5], by noticing that all programs constructed in the  $279$  proof are also contained in BFOQ.

# <sup>280</sup> **3 Circuit compilation**

 In this section, we introduce a compilation strategy for pfoq programs that strictly improves on the compilation algorithm of [\[10\]](#page-15-13). We also show that, in the bfoq fragment, circuit complexity scales in such a way that the cost of branching is the maximum cost of each branch, thereby avoiding branch sequentialization.

#### <sup>285</sup> **3.1 A new compilation algorithm**

The compilation algorithm **compile**<sup>+</sup> 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 *n* qubits. **compile**<sup>+</sup> is defined by its subroutine **compr**<sup>+</sup> (Algorithm [1\)](#page-8-0) in the following way:

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

<sup>286</sup> where P is the program to be compiled,  $[1, \ldots, n]$  is list of qubit pointers (initially all qubits),

<sup>287</sup> ⋅ is an empty control structure, and {} an empty dictionary. A *control structure* is a partial

<sup>288</sup> function in  $\mathbb{N} \to \{0,1\}$  mapping qubit pointers to their control values in a quantum case. For

289 *n* ∈ N and  $k \in \{0, 1\}$ ,  $cs[n] = k$  is the control structure obtained from *cs* by setting  $cs(n) \triangleq k$ .

290 We denote by  $dom(cs)$  the domain of the control structure. For a given  $x \in \{0,1\}^*$ , we say

291 that state  $|x\rangle$  *satisfies cs* if,  $\forall n \in dom(cs)$ ,  $cs(n) = k$  implies that  $x_n = k$ . The purpose of <sup>292</sup> control structures in the algorithm is to preserve the information of each quantum branch

<sup>293</sup> and to allow for merging using ancillas.

<span id="page-8-0"></span>Algorithm 1 ( $comp<sup>+</sup>$ ) **Input:**  $(D : S, l, cs, \text{ Anc}) \in \text{Programs} \times \mathcal{L}(\mathbb{N}) \times (\mathbb{N} \to \{0, 1\}) \times \mathcal{D}$ 1: **if**  $S =$  **skip**; **then** 

2:  $C \leftarrow \mathbb{1}$   $\triangleright$  Identity circuit 3:  $4:$  **else if**  $S = s[i] \neq U^f(j);$  and  $(s[i], l) \Downarrow_{\mathbb{N}} n$  and  $(U^f(j), l) \Downarrow_{\mathbb{C}^{2 \times 2}} M$  then 5:  $C \leftarrow M(c, [n])$   $\triangleright$  Controlled gate 6: 7: **else if**  $S = S_1 S_2$  **then** 8:  $C \leftarrow \text{compr}^+(\text{D} :: \text{S}_1, l, cs, \text{Anc}) \circ \text{compr}^+(\text{D} :: \text{S}_2, l, cs, \text{Anc})$   $\triangleright$  Composition 9: 10: **else if**  $S =$  **if** b **then**  $S_{true}$  **else**  $S_{false}$  **and**  $(b, l) \Downarrow_{\mathbb{B}} b$  **then** 11: *C* ← **compr**<sup>+</sup> (D ∶∶ S*b,l, cs,*Anc) ▷ Conditional 12: 13: **else if** S = **qcase** s[i] **of**  $\{0 \rightarrow S_0, 1 \rightarrow S_1\}$  **and**  $(s[i], l) \Downarrow_N n$  **then**  $\triangleright$  Quantum case 14:  $C \leftarrow \text{compr}^+(\text{D} :: \text{S}_0, l, cs[n := 0], \text{Anc}) \circ \text{compr}^+(\text{D} :: \text{S}_1, l, cs[n := 1], \text{Anc})$ 15: 16: **else if** S = **call** proc[i](s); **and** (s, *l*)  $\Downarrow$ <sub>*L*(N)</sub> [] **then** 17:  $C \leftarrow \mathbb{1}$ 17:  $C \leftarrow 1$   $\triangleright$  Nil call 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:  $a \leftarrow \textbf{new} \text{ ancilla}()$ 21: Anc[proc', n, |l'|]  $\leftarrow$  (*a*, *l'*); 22:  $C \leftarrow \textbf{optimize}^+(D, [(\cdot[a = 1], S^{\text{proc}}\{n/x\})], \text{proc}, l', \text{Anc})$ 23: **end if** 24: **return** C

<sub>294</sub> The aim of subroutine **compr**<sup>+</sup> is just to generate the quantum circuit corresponding <sup>295</sup> to P on *n* qubits inductively on the statement of P. When the analyzed statement is a <sup>296</sup> (possibly recursive) procedure call, **compr**<sup>+</sup> calls the **optimize**<sup>+</sup> subroutine (Algorithm [2\)](#page-9-0) to <sub>297</sub> perform an optimization of the generated quantum circuit. **optimize**<sup>+</sup> has the same inputs <sup>298</sup> as **compr**<sup>+</sup> with the addition of a list of *controlled statements*  $l_{\text{Cst}}$  and the name proc of <sup>299</sup> the procedure under analysis. A controlled statement is defined as a pair  $(c, S)$  where *cs* <sup>300</sup> is a control structure and S is a foq statement. This will allow us to generate the circuit <sup>301</sup> implementation of S (which may contain multiple gates) while keeping track of the branch <sup>302</sup> on which it is implemented.

<sup>303</sup> The compilation algorithm **compile**<sup>+</sup> is based on the process of merging procedure <sup>304</sup> calls by reasoning about the orthogonality relations within the circuit. It is similar to the <sup>305</sup> compilation algorithm **compile** of [\[10\]](#page-15-13) based on the subroutines **compr** and **optimize**, with <sup>306</sup> the differences highlighted in the code of Algorithms [1](#page-8-0) and [2:](#page-9-0) **optimize**<sup>+</sup> strictly improves <sup>307</sup> on **optimize** (Theorem [12\)](#page-11-0) by extending this analysis to procedures of different ranks.

## <sup>308</sup> **3.2 Soundness and optimization**

<sup>309</sup> The correctness of **optimize**<sup>+</sup> is a consequence of an orthogonality property between ele-<sup>310</sup> ments of the circuit being compiled that remains invariant throughout the compilation. In  $_{311}$  Algorithm [2,](#page-9-0) a recursive procedure proc is compiled by generating three separate circuits  $C_{\text{L}}$ ,  $S_{312}$  *C*<sub>M</sub>, and *C*<sub>R</sub>. The compilation process makes use of a list  $l_{\text{Cst}}$  of controlled statements which

<span id="page-9-0"></span>**Algorithm 2 (optimize**<sup>+</sup> **)** Build circuit for recursive procedure proc **Inputs:**  $(D, l_{\text{Cst}}, \text{proc}, l, \text{Anc}) \in \text{Decl} \times \mathcal{L}(\text{Cst}) \times \text{Proceedures} \times \mathcal{L}(\mathbb{N}) \times \mathcal{D}$ 

```
1: C_{\text{L}} \leftarrow 1; C_{\text{R}} \leftarrow 1; C_{\text{M}} \leftarrow 1; P \leftarrow D ∷ skip;
 2: while l_{\text{Cst}} \neq \lceil \cdot \rceil do
 3: (cs, S) \leftarrow hd(l_{\text{Cst}}); l_{\text{Cst}} \leftarrow tl(l_{\text{Cst}})4:
 5: if S = S_1 S_2 then
 6: Anc' \leftarrow Anc.copy() /* create copy of ancilla dictionary */
  7: if w_{\rm P}^{\rm proc}({\rm S}_1) = 1 then
  8: l_{\text{Cst}} \leftarrow l_{\text{Cst}} \mathbb{Q}[(cs, S_1)]; C_M \leftarrow \text{compr}^+(D : S_2, l, cs, \text{Anc}') \circ C_M9: else
10: 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}}11: end if
12: end if
13:
14: if S = if b then S<sub>true</del> <b>else S<sub>false and (b, l) \Downarrow<sub>B</sub> b then</sub></sub>
15: if w_{\text{P}}^{\text{proc}}(\text{S}_b) = 1 then
16: l_{\text{Cst}} \leftarrow l_{\text{Cst}} \mathbb{Q}[(cs, S_b)]17: else
18: C_M \leftarrow \text{compr}^+(\text{D} :: \text{S}_b, l, cs, \text{Anc}) \circ C_M19: end if
20: end if
21:
22: if S = qcase s[i] of \{0 \rightarrow S_0, 1 \rightarrow S_1\} and (s[i], l) \Downarrow_{\mathbb{N}} n then
23: if w_{\text{P}}^{\text{proc}}(S_0) = 1 and w_{\text{P}}^{\text{proc}}(S_1) = 1 then
24: l_{\text{Cst}} \leftarrow l_{\text{Cst}} \mathbb{Q}[(cs[n := 0], \mathbf{S}_0), (cs[n := 1], \mathbf{S}_1)]25: else if w_{\text{P}}^{\text{proc}}(S_1) = 0 then
26: l_{\text{Cst}} \leftarrow l_{\text{Cst}} @ [(cs[n := 0], S_0)];27: C_{\rm M} ← compr<sup>+</sup>(D ∷ S<sub>1</sub>, l, cs[n ∶= 1], Anc) ◦ C_{\rm M}28: else if w_{\text{P}}^{\text{proc}}(\text{S}_0) = 0 then
29: l_{\text{Cst}} \leftarrow l_{\text{Cst}} @ [(cs[n := 1], S_1)];30: C_{\rm M} ← compr<sup>+</sup>(D ∷ S<sub>0</sub>, l, cs[n ∶= 0], Anc) ◦ C_{\rm M}31: end if
32: end if
33:
34: if S = call proc<sup>'</sup>[i](s) and (s,l) \Downarrow<sub>L(N)</sub> l' \neq[] and (i,l) \Downarrow<sub>Z</sub> n then
35: if (\text{proc}', n, |l'|) \in \text{Anc} \textbf{ then}36: Let (a, l'') = \text{Anc}[\text{proc}', n, |l'|] in
37: e \leftarrow \textbf{new} \text{ ancilla}(); /* compatible procedure already exists: merging case */
38: C_{\text{L}} \leftarrow C_{\text{L}} \circ NOT(cs, e) \circ NOT(\cdot[e = 1], a) \circ SWAP(\cdot[e = 1], l', l'');39: C_{\text{R}} \leftarrow SWAP(\cdot [e = 1], l'', l') \circ NOT(\cdot [e = 1], a) \circ NOT(xs, e) \circ C_{\text{R}}40: else
41: a \leftarrow \textbf{new} \text{ ancilla}() /* no compatible procedure: create new ancilla */
42: Anc[proc', n, |l'|] ← (a, l');
43: C_{\text{L}} \leftarrow C_{\text{L}} \circ NOT(cs, a); C_{\text{R}} \leftarrow NOT(cs, a) \circ C_{\text{R}};44: l_{\text{Cst}} \leftarrow l_{\text{Cst}} \mathbb{Q}[(\cdot[a=1], \text{S}^{\text{proc}'}\{n/\text{x}\})]45: end if
46: end if
47: end while
48: return C_{L} \circ C_{M} \circ C_{R}
```
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 $_{313}$  have not yet been compiled. Given a program P and an input procedure proc, the list  $l_{\text{Cst}}$ contains controlled statements  $(c, S)$  such that  $w_P^{\text{proc}}(S) = 1$ , whereas  $C_M$  contains circuits <sup>315</sup> for statements such that  $w_P^{\text{proc}}(S) = 0$  but that are nonetheless orthogonal to those in  $l_{\text{Cst}}$ , for 316 which merging will be possible. Circuits  $C_{\text{L}}$  and  $C_{\text{R}}$  contain circuits for statements for which <sup>317</sup>  $w_P^{\text{proc}}(S) = 0$  and that are not orthogonal to the elements of *l*<sub>Cst</sub>. The circuit below pictures 318 how the output circuit is generated from the circuits  $C_L$ ,  $C_M$ , and  $C_R$  and the list  $l_{\text{Cst}}$ .





<sup>320</sup> The steps of **optimize**<sup>+</sup> are depicted in Figure [7,](#page-11-1) where in each case we treat a controlled 321 statement  $(cs, S) \in l_{\text{Cst}}$ . A gate placed inside the violet box  $\Box$  denotes the new controlled 322 statement that replaces  $(c, S)$  in  $l_{\text{Cst}}$ . A gate placed inside a grey box  $\Box$  indicates a circuit  $323$  that is compiled and added to  $C_M$ . The notation is agnostic to the precise placement of  $324$  these objects within  $l_{\text{Cst}}$  and  $C_M$ , making use of the orthogonality relation described in <sup>325</sup> Lemma [11](#page-10-0) which renders the choice inconsequential. Figures [7a, 7b,](#page-11-1) and [7c](#page-11-1) contain two <sup>326</sup> circuits consisting of the different possible cases of compilation:

 $327$  In Figure [7a,](#page-11-1) we consider a sequence  $S_1 S_2$ . This includes the case where  $S_2$  is recursive  $328$  (left) and the one where S<sub>1</sub> is recursive (right). Given the WIDTH<sub>≥1</sub> condition, there are <sup>329</sup> no more cases.

 $\mathbf{I}$  In Figure [7b,](#page-11-1) the case of classical control, we have the step where  $S_b$  contains a recursive <sup>331</sup> call (above) and where it does not (below).

 $332 \equiv$  For the case of quantum branching (Figure [7c\)](#page-11-1), 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).

<sup>334</sup> Finally, we consider the case of a procedure call. Either there is already a compatible <sup>335</sup> procedure and merging is performed (Figure [7d\)](#page-11-1) or a new ancilla is used to anchor the <sup>336</sup> procedure (Figure [7e\)](#page-11-1).

<sup>337</sup> We formalize orthogonality between controlled statements as follows.

<sup>338</sup> ▶ **Definition 10** (Orthogonality between control structures)**.** *We say that two control structures are orthogonal, also denoted cs* ⊥ *cs*′ *, if* ∃*i* ∈ N *such that i* ∈ *dom*(*cs*) ∩ *dom*(*cs*′ <sup>339</sup> ) *and where*  $c s(i) + c s'(i) = 1.$ 

<sup>341</sup> Hence, two control structures are orthogonal if there is no base state that satisfies them both. <sup>342</sup> We now show that the steps of **optimize**<sup>+</sup> respect an orthogonality invariant.

<span id="page-10-0"></span>343 **► Lemma 11** (Orthogonality invariant). At each step of the subroutine optimize<sup>+</sup>, the list  $\frac{1}{244}$  *l*<sub>Cst</sub> *and the circuit*  $C_M$  *satisfy the following properties:* 

 $\frac{1}{345}$  **1.** All controlled statements in  $l_{\text{Cst}}$  are mutually orthogonal:

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

 $347$  **2.** Any controlled statement in  $l_{\text{Cst}}$  commutes with any element of  $C_M$ :

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

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

351 We now prove by induction that it is an invariant. Let  $(c, S) \in l_{\text{Cst}}$  be the controlled 352 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,  $(cs, S)$ 

<span id="page-11-1"></span>

(d)  $S = \text{call proc}'[i](s);$  (merging).



Figure 7 A step of the optimize<sup>+</sup> subroutine.

353 is replaced with  $(c, S_1)$  in  $l_{\text{Cst}}$  and  $C_M$  is unchanged – therefore, the invariant property <sup>354</sup> remains true. The case where  $w_P^{\text{proc}}(S_1) = 0$  and  $w_P^{\text{proc}}(S_2) = 1$  is analogous.

If  $S = \textbf{if } b \textbf{ then } S_0 \textbf{ else } S_1$ , then consider the case  $(b, l) \Downarrow_B 0$ , where if  $w_P^{\text{proc}}(S_0) = 1$  we <sup>356</sup> have that  $(c, S)$  is replaced with  $(c, S_0)$  in  $l_{\text{Cst}}$  and  $C_M$  remains the same, and therefore <sup>357</sup> the property remains true. If  $w_{\rm P}^{\rm proc}({\rm S}_0) = 0$  we have that  $(cs, S)$  is removed from  $l_{\rm Cst}$  and <sup>358</sup>  $C_M \leftarrow [[cs, S)] \circ C_M$ . By the induction hypothesis all other  $cs_i$  in  $l_{\text{Cst}}$  are orthogonal to  $cs$ 359 and therefore the property is conserved. The same can be shown for the case of  $(b, l) \downarrow_{\mathbb{B}} 1$ .

 $\mathbf{S} = \mathbf{q} \cdot \mathbf{c} \cdot \mathbf{s} \cdot \mathbf{d} \cdot \mathbf{s} = \mathbf{q} \cdot \mathbf{c} \cdot \mathbf{s} \cdot \mathbf{s}$  $\text{c}$ <sub>261</sub>  $\text{to}$   $\text{c}$   $\text{c}$  <sup>362</sup> all cases preserve the condition.

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

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

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

<span id="page-11-0"></span><sup>369</sup> We now show that algorithm **compile**<sup>+</sup> strictly improves on the asymptotic size of circuit, <sup>370</sup> compared to the **compile** algorithm of [\[10\]](#page-15-13).

**• Theorem 12.** For any PFOQ program P,  $\#\text{compile}^+(P,n) = O(\#\text{compile}(P,n))$ . Fur $t_{372}$  thermore, there exist programs for which  $\#\textbf{compile}^+(\text{P}, n) = o(\#\textbf{compile}(\text{P}, n))$ .

<sup>373</sup> **Proof.** The circuit size in both cases is asymptotically bounded by the number of ancillas <sup>374</sup> created. Since we do more merging than before the result follows. Table [1](#page-13-0) provides some  $375$  examples to show the second claim.

<span id="page-12-0"></span> $\text{376}$  ▶ Theorem 13 (No branch sequentialization). For P ∈ BFOQ and  $n \in \mathbb{N}$ ,  $\#\textbf{compile}^+(\text{P}, n) = \text{176}$  $377 \quad O(\text{level}_{P}(n)).$ 

**Proof.** The theorem can be shown by structural induction on the program body, by checking <sup>379</sup> that it is the case in each scenario that the circuit size scales with the level of the program. <sup>380</sup> All cases are straightforward except the one of the quantum control case, which is proven at <sup>381</sup> the end. The BASIC restrictions give us the following two properties during the compilation: <sup>382</sup> (a) merging can be done in constant time, since there is no need for controlled-swap gates, 383 and (b) a call to a recursive function only result in at most  $O(n)$  calls to procedures of the <sup>384</sup> same rank with unique ancillas.

<sup>385</sup> We proceed by structural induction on the program body, considering that the statement <sup>386</sup> is part of a procedure call for procedure proc.

 $\mathbf{s}$ <sup>387</sup> (S = **skip**; or S =  $\bar{q}[i]$  \*= U;) in this case we have that, level<sub>p</sub> $(n) = 0$  and the the circuit is <sup>388</sup> of constant size.

 $\mathcal{S}_3$   $\cong$   $(S = S_1 S_2)$  In this case,  $S_1$  and  $S_2$  are compiled in series (Figure [7a\)](#page-11-1). The size of the  $\frac{390}{2}$  circuit for S is then given by the sum of the sizes of the circuits of S<sub>1</sub> and S<sub>2</sub>, and by <sup>391</sup> definition the level of S is the sum of the levels.

 $392 \equiv (S = \textbf{if } b \textbf{ then } S_0 \textbf{ else } S_1)$  Depending on the value of b the circuit for S either it  $393$  corresponds to the circuit for  $S_0$  or  $S_1$ . Therefore the size of the circuit is bounded by <sup>394</sup> the maximum of between the two statements, as in the definition of level.

 $\mathcal{S}$  =  $(S = \text{call proc[i]}(s))$  This case also follows the definition of level since the circuit size is <sup>396</sup> the one given inductively by the non-procedure-call operations (constant size) plus the <sup>397</sup> 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.

 $402$  The base case is given by (b), therefore we may consider  $r > 1$ . For the inductive case, we <sup>403</sup> consider three possible scenarios:

<sup>404</sup>  $w_{\text{proc}}^{\text{P}}(S_0) = w_{\text{proc}}^{\text{P}}(S_1) = 0$ . Therefore, S<sub>0</sub> and S<sub>1</sub> 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.

 $w_{\text{proc}}^{\text{P}}(S_0) = w_{\text{proc}}^{\text{P}}(S_1) = 1$ . In this case,  $S_0$  and  $S_1$  are of the same rank, *r*, and all <sup>409</sup> their procedure calls may be merged. Therefore, the asymptotic number of such calls is 410 bounded between the maximum between  $S_0$  and  $S_1$  (consider that, if there is no overlap <sup>411</sup> between the ancillas needed, their number is still bounded linearly). Applying the IH on <sup>412</sup> the procedures of rank  $r - 1$  we obtain the desired result.

 $w_{\text{proc}}^{\text{P}}(S_0) = 0$  and  $w_{\text{proc}}^{\text{P}}(S_1) = 1$ . Therefore,  $S_0$  contains calls to procedures of rank  $r' < r$ whereas  $S_1$  contains calls to procedures of rank *r*. The number of procedures of rank  $r'$ 414 <sup>415</sup> is bounded asymptotically by the maximum between those in  $S_0$  and  $S_1$ , therefore we  $416$  obtain our result.

<span id="page-13-0"></span>

**Table 1** Circuit size complexity bounds given by the compilation strategy in [\[10\]](#page-15-13) and **compile**<sup>+</sup> described in this work. For all of these problems, we give the corresponding programs in BFOQ.

# <sup>417</sup> **4 Examples**

<sup>418</sup> In this section, we provide several examples illustrating our results, including general examples <sup>419</sup> on regular expressions. We show that any regular language can be decided by a BFOQ program <sup>420</sup> whose compiled quantum circuit of linear size (Theorem [17\)](#page-14-2). A benchmark, illustrating the <sup>421</sup> difference between our compilation algorithm and the one in [\[10\]](#page-15-13), is provided in Table [1.](#page-13-0)

#### <span id="page-13-1"></span><sup>422</sup> ▶ **Example 14** (Palindromes)**.** Consider the following bfoq program PALINDROME.

- $_1$  **decl** palindrome( $\bar{q}$ ){ 2 **if**  $|\bar{q}| > 2$  **then** 3 **qcase**  $\bar{q}[1, |\bar{q}|-1]$  **of** { 4 00 → **call** palindrome( $\bar{q} \ominus [1, -2]$ );  $5 \qquad \qquad 01 \rightarrow \mathbf{skip};$ 6  $10 \rightarrow$  **skip**; 7 11 → **call** palindrome( $\bar{q} \ominus [1, -2]$ ); 423
	- 8 } 9 **else**  $\bar{q}[-1]$  **\*=** NOT; }
	- $10$   $\therefore$  **call** palindrome( $\bar{q}$ );
- 424

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  $\epsilon$  width $\epsilon_1$  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  $\bar{q} \ominus [1, |\bar{q}|-1]$ , we conclude that it is also in bfoq. We are therefore in a position to apply Theorem [13.](#page-12-0)

 $\text{425}$  Since  $rk(\text{PALINDROME}) = rk_{\text{PALINDROME}}(\text{palindrome}) = 1$ , by Lemma [7,](#page-6-2) we obtain the conclusion that  $\#\text{optimize}^+(P,n) = O(n)$ , i.e., the compilation procedure generates  $_{427}$  a circuit of size linear on the input. Indeed, for PALINDROME, **compile**<sup>+</sup> generates the <sup>428</sup> following circuit in the case where *n* is even:





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

<span id="page-14-0"></span> **► Example 15** (Chained substring). Let  $s_0 = 001$  and  $s_1 = 11$ . Let  $\mathcal{L}$  be the regular language defined by identifying strings containing an instance of *s*<sup>0</sup> followed eventually by an instance of *s*<sup>1</sup> in a word, i.e., the language defined by the regular expression ∗*s*<sup>0</sup> ∗ *s*1∗. We can define 435 a BFOQ program (Appendix [C\)](#page-19-0) that detects inputs in  $\mathcal L$  using the following call graph:



<sup>437</sup> The program has as body a procedure call **call**  $f_0(\bar{q})$ ; and consists of 5 procedures  $f_i$  and a terminating procedure  $\oplus$ . An arrow  $s \to^b t$  with  $b \in \{0,1\}$  indicates a procedure call of the <sub>439</sub> form **call**  $t(\bar{q} \ominus [1])$ ; appears in the body of procedure *s* done in a branch with  $\bar{q}[1]$  in state *b*. 440 The maximum rank of a procedure is 3 (for  $f_0$  and  $f_1$ ) and the circuit obtained by the  $\text{441}$  technique in [\[10\]](#page-15-13) gives a circuit of size  $\Theta(n^3)$ . On the other hand, the size of the circuit <sup>442</sup> produced by **compile**<sup>+</sup> grows linearly on the input size.

<sup>443</sup> In the previous example, the bound obtained by **compile**<sup>+</sup> 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.](#page-12-0)

<span id="page-14-3"></span>**← Definition 16.** Let  $A: \{0,1\}^*$  →  $\{0,1\}$  be a decision problem. Given a FOQ program P, we *say that* P decides *A if, for*  $\bar{x}$  ∈ {0*,* 1}<sup>\*</sup> and  $y$  ∈ {0*,* 1}*, we have that*  $[$ P $]$ ( $|\bar{x}y$ ) =  $|\bar{x}(y \oplus A(\bar{x}))$ *)*.

<span id="page-14-2"></span> ▶ **Theorem 17** (Regular languages)**.** *For any regular language* L*, there exists a* bfoq *program*  $\mathcal{F}_{\mathcal{A}}$ <sup>50</sup> P that decides if  $\bar{x} \in \mathcal{L}$ , for any  $\bar{x} \in \{0,1\}^*$ , such that  $\#\textbf{compile}^+(\mathrm{P},n) \in O(n)$ .

**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.](#page-14-3) Since  $\mathcal D$  is deterministic, the level of the corresponding program is bounded linearly. Using Theorem [13](#page-12-0) we obtain the desired result. ◀

<span id="page-14-1"></span> $\bullet$  **Example 18.** Let SUM<sub>r</sub> be the decision problem of checking if an input bitstring contains precisely *r* 1s. This corresponds to identifying bitstrings in the regular expression  $(0^*1)^r0^*$  and therefore, by Theorem [17,](#page-14-2) there exists a BFOQ program deciding  $SUM<sub>r</sub>$  such that 458 **compile**<sup>+</sup> 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 <sup>461</sup> quantum programming language with quantum control of [\[10\]](#page-15-13). We have shown that BFOQ is sound and complete for polynomial time computation (Theorem [9\)](#page-7-0) and that the branch sequentialization problem introduced by [\[19\]](#page-15-14) is solved for bfoq programs: the compiled circuit has size upper-bounded by the maximal complexity of program branches (Theorem [13\)](#page-12-0). As a consequence, the compilation procedure generates circuits with a better size complexity than the compilation algorithm of [\[10\]](#page-15-13) (Theorem [12\)](#page-11-0). This result and the expressivity of bfoq are illustrated by the Examples of Table [1.](#page-13-0) A future and challenging research direction includes the extension of this work to higher-order.

<span id="page-15-18"></span><span id="page-15-17"></span><span id="page-15-16"></span><span id="page-15-15"></span><span id="page-15-14"></span><span id="page-15-13"></span><span id="page-15-12"></span><span id="page-15-11"></span><span id="page-15-10"></span><span id="page-15-9"></span><span id="page-15-8"></span><span id="page-15-7"></span><span id="page-15-6"></span><span id="page-15-5"></span><span id="page-15-4"></span><span id="page-15-3"></span><span id="page-15-2"></span><span id="page-15-1"></span><span id="page-15-0"></span>

<span id="page-16-0"></span>

# <sup>517</sup> **A Semantics of FOQ programs**

 $\sum_{s=18}$  In Section [2,](#page-3-1) we have defined  $\mathcal{L}(N)$  as the set of lists of natural numbers  $[n_1, \ldots, n_k]$  (the <sup>519</sup> empty list being denoted by []), which are used to represent list of (unique) qubit pointers <sup>520</sup> in the semantics.

<sup>521</sup> *Basic data types τ* are interpreted as follows:



525 Each basic operation op ∈ {+,-, >, ≥, =, ∧, ∨, ¬} of arity *n*, with  $1 \le n \le 2$ , has a type  $\frac{1}{226}$  signature  $\tau_1 \times \ldots \times \tau_n \to \tau$  fixed by the program syntax. For example, the operation + has signature Integers × Integers → Integers. A total function  $[\![op]\!] \in [\![\tau_1]\!] \times \ldots \times [\![\tau_n]\!] \to [\![\tau]\!]$  is<br>sassociated to each basic operation op. associated to each basic operation op.

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

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

where  $\tilde{\mathbb{C}}$  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  $\text{S32}$  matrix *M* satisfies  $M^* \circ M = M \circ M^* = I$ , with  $M^*$  being the conjugate transpose of *M* and <sup>533</sup> *I* being the identity matrix.

For each basic type  $\tau$ , the reduction  $\psi_{\llbracket \tau \rrbracket}$  is a map in  $\tau \times \mathcal{L}(\mathbb{N}) \to \llbracket \tau \rrbracket$ . Intuitively, it maps 535 an expression of type  $\tau$  to its value in  $\llbracket \tau \rrbracket$  for a given list *l* of pointers in memory. These<br>536 reductions are defined in Figure 8, where e and d denote either an integer expression i or a <sup>536</sup> reductions are defined in Figure [8,](#page-16-1) where e and d denote either an integer expression i or a <sup>537</sup> Boolean expression b.

<span id="page-16-1"></span>
$$
\frac{(e, l) \Downarrow_{\lceil\tau_{1}\rceil} m \quad (d, l) \Downarrow_{\lceil\tau_{2}\rceil} n}{(e \text{ op } d, l) \Downarrow_{\lceil\text{op}\rceil(\lceil\tau_{1}\rceil, \lceil\tau_{2}\rceil)} \lceil\text{op}\rceil(m, n)} \quad (Op) \qquad \frac{(i, l) \Downarrow_{\mathbb{Z}} n}{(U^{f}(i), l) \Downarrow_{\mathbb{C}^{2 \times 2}} \lceil\text{U}^{f}\rceil(n)} \quad (Unit)
$$
\n
$$
\frac{(e, l) \Downarrow_{\lceil\text{op}\rceil(\lceil\tau_{1}\rceil, \lceil\tau_{2}\rceil)} \lceil\text{op}\rceil(m, n)}{(s, l) \Downarrow_{\mathcal{L}(N)} \lceil x_{1}, \ldots, x_{m}\rceil} \quad (i, l) \Downarrow_{\mathbb{Z}} k \in [1, m]} \quad (Rm_{\epsilon})
$$
\n
$$
\frac{(s, l) \Downarrow_{\mathcal{L}(N)} \lceil x_{1}, \ldots, x_{n-1}, x_{k+1}, \ldots, x_{m}\rceil}{(s, l) \Downarrow_{\mathcal{L}(N)} \lceil x_{1}, \ldots, x_{m-1}, x_{k+1}, \ldots, x_{m}\rceil} \quad (i, l) \Downarrow_{\mathbb{Z}} k \notin [1, m]} \quad (Rm_{\epsilon})
$$
\n
$$
\frac{(s, l) \Downarrow_{\mathcal{L}(N)} \lceil x_{1}, \ldots, x_{m}\rceil \quad (i, l) \Downarrow_{\mathbb{Z}} k \in [1, m]}{(s, l) \Downarrow_{\mathcal{L}(N)} \lceil x_{1}, \ldots, x_{m}\rceil} \quad (i, l) \Downarrow_{\mathbb{Z}} k \in [1, m]} \quad (Rm_{\epsilon})
$$
\n
$$
\frac{(s, l) \Downarrow_{\mathcal{L}(N)} \lceil x_{1}, \ldots, x_{m}\rceil \quad (i, l) \Downarrow_{\mathbb{Z}} k \in [1, m]}{(s, l) \Downarrow_{\mathbb{Z}} n} \quad (Qu_{\epsilon})
$$
\n
$$
\frac{(s, l) \Downarrow_{\mathcal{L}(N)} \lceil x_{1}, \ldots, x_{m}\rceil \quad (i, l) \Downarrow_{\mathbb{Z}} k
$$

**Figure 8** Semantics of expressions

Recall from Section [2](#page-3-1) that the set of *configurations* over *n* qubits, denoted Conf<sub>*n*</sub>, is defined by

Conf<sub>n</sub>  $\triangleq$  (Statements ∪ { $\tau$ ,  $\bot$ }) ×  $\mathcal{H}_{2^n}$  ×  $\mathcal{P}(\mathbb{N})$  ×  $\mathcal{L}(\mathbb{N})$ *,* 

538 where  $\mathcal{P}(\mathbb{N})$  being the powerset over N and where  $\top$  and  $\bot$  are two special symbols for <sup>539</sup> termination and error, respectively. Let ◇ stand for a symbol in {⊺*,* }.

540 A configuration  $c = (S, |\psi\rangle, \mathcal{S}, l) \in \text{Conf}_n$  contains a statement S to be executed (provided  $\mathfrak{f}_{541}$  that  $S \notin \{\top, \bot\}$ , a quantum state  $|\psi\rangle$  of length *n*, a set S containing the qubit pointers that <sup>542</sup> are allowed to be accessed by statement S, and a list *l* of qubit pointers.

 $_{543}$  The program big-step semantics  $\longrightarrow$ , described in Figure [9,](#page-17-0) is defined as a relation in  $\cup_{n\in\mathbb{N}}$  Conf<sub>n</sub> ×  $\mathbb{N}$  × Conf<sub>n</sub>.

<span id="page-17-0"></span>
$$
\frac{\left(\text{skip}, \psi\right), \mathcal{S}, l\right) \xrightarrow{\mathbf{0}} \left(\text{r}, \psi\right), \mathcal{S}, l\right)}{\left(\text{s}[i], l\right) \Downarrow_{\mathbb{N}} n \notin \mathcal{S}} \quad \text{(Asg.)} \quad \text{(Asg.)} \quad \text{(Asg.)} \quad \text{(Bsg.)} \quad \text{(Csg.)} \quad \text{(Dsg.)} \quad \text{(Dsg
$$

**Figure 9** Semantics of statements

# <sup>545</sup> **B Proofs**

<sup>546</sup> In this section, we provide the full proof of Theorem [17.](#page-14-2) Towards that end, we first define a <sup>547</sup> notion of call-graph.

**548**  $\blacktriangleright$  **Definition 19** (Call graph). *A* call graph G *is a triple* (proc,  $V, E$ ) *where* 

 $\mathcal{F}_{\text{549}}$  proc  $\in V$  *is the entry node*;

 $V \subseteq$  Procedures *is a set of nodes containing a special procedure*  $\oplus$ ;

 $E = E \subseteq V \times L \times V$  *is a set of labeled directed edges, where labels correspond to combinations* <sup>552</sup> *of quantum and classical conditionals.*

 $553$  *Procedure*  $\oplus$  *only applies a NOT gate to the last qubit in the input and terminates. Labels* L <sup>554</sup> *are defined as follows: values* {0*,* 1} *denote a quantum if statement on the first qubit, and*  $\overline{q}| = n$  *or*  $|\overline{q}| > n$  *denotes a boolean condition on the size of the input.* 

556 **• Theorem 17** (Regular languages). For any regular language  $\mathcal{L}$ , there exists a BFOQ program  $\mathcal{F}$ <sup>557</sup> P that decides if  $\bar{x} \in \mathcal{L}$ , for any  $\bar{x} \in \{0,1\}^*$ , such that  $\#\textbf{compile}^+(\mathrm{P},n) \in O(n)$ .

**Proof.** Let  $D$  be a deterministic finite automaton deciding  $\mathcal{L}$ . We will construct the PFOQ program P by using  $D$  to define the call graph for P. The subtlety in the transformation  $\frac{560}{100}$  is in the difference between the acceptance condition in D (i.e., termination in an accept state) and the *acceptance nodes* of the call graph, referring here to the ⊕ nodes. For a base 562 state  $|\bar{xy}\rangle$ , the program P outputs  $|\bar{x}(-y)\rangle$  iff it *ever* reaches a ⊕ node, at which point P terminates.

<sup>564</sup> The call graph is then defined as follows. The call graph contains a node for each state of  $\frac{1}{565}$  C, with the same transitions, except for those that constitute incoming our outgoing edges of  $\alpha$  an accept state, i.e., edges  $x_i, y_i, z_i$  in the following diagram:



567

<sup>568</sup> 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  $i = 1 \ldots m$ , we denote by  $\{c_i\}_{i=1 \ldots m}$  a set of  $m$  edges each labelled with a conditions  $c_i$ .

<sup>575</sup> Since each procedure performs at most one procedure call per branch (recursive or  $576$  otherwise) its level will be linear on the input size.

# <span id="page-19-0"></span><sup>577</sup> **C Regular languages (Example [15\)](#page-14-0)**

<sup>578</sup> The following is the program defined by the call graph given in Example [15.](#page-14-0)

```
579 1 decl f_0(\bar{q}){
580 2 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])\},\581
582 3 decl f_1(\bar{q}){
583 4 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])\},\584
585 5 \text{ decl } f_2(\bar{q})586 6 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])\},\587
588 7 decl f_3(\bar{q}){
589 8 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])\},\590
591 9 decl f_4(\bar{q}){
592 10 qcase \bar{q}[1] of \{0 \rightarrow \text{call } f_3(\bar{q} \ominus [1]), 1 \rightarrow \text{call } \oplus (\bar{q} \ominus [1])\},\593
594 11 decl \oplus (\bar{q}){
595 12 \bar{q}[-1] *= NOT; }
596
            13 : call f_0(\bar{q});
598
```
<sup>599</sup> It is straightforward to verify that all conditions of bfoq are met and that the level of <sup>600</sup> the program is linearly bounded.