

Quantum Branching Programs and Space-Bounded Nonuniform Quantum Complexity

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Abstract. In this paper, the space complexity of nonuniform quantum algorithms is investigated using the model of quantum branching programs (QBPs). In order to clarify the relationship between QBPs and nonuniform quantum Turing machines, simulations between these two models are presented which allow to transfer upper and lower bound results. Exploiting additional insights about the connection between the running time and the precision of amplitudes, it is shown that nonuniform quantum Turing machines with algebraic amplitudes and QBPs with a suitable analogous set of amplitudes are equivalent in computational power if both models work with bounded or unbounded error. Furthermore, quantum ordered binary decision diagrams (QOBDDs) are considered, which are restricted QBPs that can be regarded as a nonuniform analog of one-way quantum finite automata. Upper and lower bounds are proved that allow a classification of the computational power of QOBDDs in comparison to usual deterministic and randomized variants of the model. Finally, an extension of QBPs is proposed where the performed unitary operation may depend on the result of a previous measurement. A simulation of randomized BPs by this generalized QBP model as well as exponential lower bounds for its ordered variant are presented.

1. Introduction

The intriguing open question behind the research on quantum computing is whether there are problems that can be solved more efficiently by quantum computers than by classical ones. Shor's famous quantum algorithm for factoring integers in polynomial time [35] provides the most conclusive evidence so far in favor of an affirmative answer of this question. The notion of a quantum algorithm is made precise by models of computation such as quantum Turing machines (QTMs), quantum circuits, quantum finite automata (QFAs), and quantum communication protocols. For an introduction to these models, we refer to the textbooks of Gruska [13], Kitaev, Shen, and Vyalys [18], and Nielsen and Chuang [26].

Apart from the obviously important computation time, different other complexity measures for quantum algorithms have been investigated. Space is a crucial resource due to inherent technical constraints in the current physical realizations of quantum computers. As pointed out by Ambainis and Freivalds [7], the goal of obtaining systems with a small quantum mechanical part was one of the motivations for considering quantum finite automata. In his seminal paper [39] and its later extensions [40, 41], Watrous investigated the space complexity of quantum algorithms in the more general model of quantum Turing machines. The quantum Turing machines considered by Watrous may have algebraic transition amplitudes and are unidirectional, i. e.,

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the direction of the head movements is a function of the state entered in a computation step. Among other results, he has shown for this scenario that space $O(s)$ probabilistic Turing machines with unbounded error and quantum Turing machines with unbounded error are equivalent in computational power, where s is a space-constructible function. It is open whether similar statements hold for other types of error, e. g., bounded error. It is also not known whether the requirement of algebraic transition amplitudes is crucial for space-restricted quantum Turing machines, despite the results of Adleman, DeMarrais, and Huang [3] that allow us to restrict the set of amplitudes to $\{0, \pm 3/5, \pm 4/5, \pm 1\}$ for polynomial time, bounded error quantum Turing machines. Finally, even the standard assumption of unidirectionality remains to be justified for QTMs with sublinear space-bounds, since the known simulations for the time-bounded case due Bernstein and Vazirani [11] and Yao [43] or Nishimura and Ozawa [27] can not be applied in an obvious way.

Already classical Turing machines have turned out to be a quite cumbersome device for proving upper and lower bounds. Branching programs are a graphic representation of boolean functions and as such are more amenable to combinatorial arguments than Turing machines. Furthermore, it is well-known that the logarithm of the size of branching programs is asymptotically equal to the space complexity for the nonuniform (advice taking) variant of Turing machines (Cobham [12], Pudlák and Žák [30]). Recently obtained lower bound results for branching programs [8, 5, 6, 9, 10], which imply time-space tradeoffs for sequential computations, underline the significance of branching programs in the investigation of space complexity.

In this paper we deal with a quantum variant of branching programs. In order to give a feeling of how quantum branching programs (QBPs) work, we consider the example in Figure 1. For the formal definition and the technical details we refer to Definitions 2.4 and 2.5. The QBP in the figure represents a boolean function depending on the variables x_1 and x_2 . Each node $v \in V = \{v_1, \dots, v_6\}$ of the QBP is associated with a vector $|v\rangle$ of an orthonormal basis of the Hilbert space $\mathcal{H} = \mathbb{C}^{|V|}$. Each intermediate state of the computation of the QBP is a vector in \mathcal{H} . The initial state of the QBP is $|v_1\rangle$, where v_1 is the start node of the QBP. Each computation step consists of a first phase, where a projective measurement is used to decide whether the computation continues or whether it stops with the result 0 or 1, and a second phase, where a unitary transformation described by the edge labels is applied to the state. If $x_i = 0$ ($x_i = 1$), only the dashed (solid) edges leaving each x_i -node contribute to this transformation. In our example the projections describing the measurement are $E_{\text{cont}} = |v_1\rangle\langle v_1| + \dots + |v_4\rangle\langle v_4|$, $E_0 = |v_5\rangle\langle v_5|$, and $E_1 = |v_6\rangle\langle v_6|$, i. e., the projections on the subspaces spanned by the vectors corresponding to interior nodes and sinks labeled by 0 and 1, resp. Assume that $x_1 = x_2 = 0$. The initial state is $|v_1\rangle$. The projective measurement yields that the computation is continued with probability 1. The dashed edges leaving v_1 are labeled by $1/\sqrt{2}$, hence, the next state is $(1/\sqrt{2})(|v_2\rangle + |v_3\rangle)$. In the second step the computation again continues with probability 1 and according to the labels of the edges leaving v_2 and v_3 the next state is $|v_6\rangle$. Hence, in the third step the computation stops with probability 1 and the result is 1.

The most important complexity measures for QBPs are the size of the QBP, i. e., its number of nodes, and the (expected or worst-case) computation time. QBPs may be cyclic or acyclic. For acyclic QBPs one can furthermore consider the width of the QBP, i. e., the maximum number of nodes with the same distance from the start node. Before we present our results on the relationship between the complexity measures for QBPs and other complexity measures for boolean functions, in particular the space complexity of quantum Turing machines, we discuss previous work on QBPs.

Ablyayev, Gainutdinova, and Karpinski [1] and Nakanishi, Hamaguchi, and Kashiwabara [24] have introduced quantum OBDDs (quantum ordered binary decision diagrams), i. e., acyclic

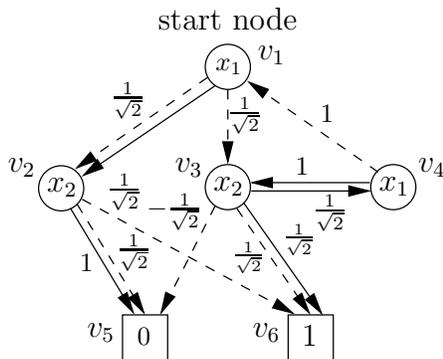


Figure 1: An example of a QBP.

QBPs where the input variables may only be read once in a fixed order during each computation. Ablayev, Gainutdinova, and Karpinski have presented a function that requires linear width in the input length for deterministic OBDDs, but only logarithmic width for quantum OBDDs. Nakanishi, Hamaguchi, and Kashiwabara have obtained a similar gap, but their lower bound even holds for randomized OBDDs. More recently, Ablayev, Moore, and Pollett [2] have proved that the class of functions that can be exactly computed by oblivious width-2 QBPs of polynomial size coincides with the class NC^1 , while width 5 is necessary classically unless $\text{NC}^1 = \text{ACC}$. Finally, Špalek [37] has studied a general model of QBPs and has independently come up with a definition similar to that used here. Furthermore, he has also presented exact simulations between QBPs whose transition function is composed of unitary matrices from a finite basis and quantum Turing machines defined analogously. In the following, we describe the contributions of our paper. For the sake of a clearer presentation, we group the results into three parts.

First Part: Simulations (Sections 2–5). In Sections 2 and 3 we define quantum branching programs and extend the definition of quantum Turing machines (QTMs) to the nonuniform case. Following Watrous [39, 40, 41], we include unidirectionality as a part of our definition of QBPs and we usually consider unidirectional nonuniform QTMs. Simulations between QBPs and unidirectional nonuniform QTMs are presented in Section 4. Our first result shows that unidirectional nonuniform QTMs using space $O(\log S)$ can be simulated by QBPs of size $\text{poly}(S)$ taking the same number of computation steps as the simulated machine. In the opposite direction, we obtain an approximate simulation of QBPs of size S by unidirectional nonuniform QTMs that carry out T simulation steps with approximation error ε in space $\text{poly}(S + \log \log(T/\varepsilon))$ and time $\text{poly}(S, T, \log(1/\varepsilon))$. These results are for QBPs and QTMs whose amplitudes are arbitrary complex numbers.

As remarked above, the standard set of transition amplitudes for QTMs in the space-bounded scenario are algebraic numbers. As an analogous standard set for QBPs we propose short amplitudes, i. e., amplitudes that can be represented in polynomial bit length in the size of the QBP as rational polynomials on finitely many algebraic numbers. Using our general simulation results and additional insights about the connection between running time and the precision of amplitudes, we show that in the case of bounded and unbounded error, QBPs with short amplitudes and size $\text{poly}(S)$ and unidirectional nonuniform QTMs with algebraic amplitudes using space $O(\log S)$ are of the same computational power.

In Section 5, we justify our standard assumption of unidirectionality for the considered models. We provide a space-efficient approximate simulation of (general) nonuniform QTMs by unidirectional ones. In particular, this result yields that $O(\log S)$ space nonuniform QTMs, $O(\log S)$

space unidirectional nonuniform QTMs, and $\text{poly}(S)$ size QBPs are of the same computational power if these models work with algebraic and short amplitudes, resp., and with bounded or unbounded error. Altogether, these arguments show that QBPs are a suitable model for exploring space-bounded nonuniform quantum complexity.

Second Part: QOBDDs (Section 6). We explore the relationship between the size of quantum OBDDs (QOBDDs) and classical OBDDs. First, we design polynomial size QOBDDs for a function that classical deterministic OBDDs can only represent in exponential size, as well as for a partially defined function for which even randomized OBDDs require exponential size. On the other hand, even very simple functions can be hard for QOBDDs. We show that for the disjointness function $(\bar{x}_1 \vee \bar{x}_2) \wedge (\bar{x}_3 \vee \bar{x}_4) \wedge \cdots \wedge (\bar{x}_{n-1} \vee \bar{x}_n)$ as well as the inner product function $x_1x_2 \oplus x_3x_4 \oplus \cdots \oplus x_{n-1}x_n$, QOBDDs require exponential size, while deterministic OBDDs can represent these functions in linear size. Finally, we prove that zero error QOBDDs of polynomial size are no more powerful than polynomial size reversible OBDDs.

Third Part: QBPs with Generalized Measurements (Section 7). For quantum OBDDs as well as for quantum finite automata, the unitarity requirement of quantum algorithms is a serious restriction. Intuitively, the problem is that it is difficult in these models to forget input already read. In Section 7 we study the question of whether it may help to allow measurements to choose the unitary transformation for the next computation step (apart from checking whether the computation has stopped). For quantum circuits this question has already been considered by Aharonov, Kitaev and Nisan [4], who have proposed to describe the states and the computations of quantum circuits by mixed states and superoperators, resp. We define natural variants of QBPs and QOBDDs with generalized measurements and investigate some of their properties. QBPs and QOBDDs with generalized measurements can simulate their randomized counterpart without increase in size. On the other hand, we prove an exponential lower bound on the size of QOBDDs with generalized measurements for all so-called k -stable functions. This class includes, e. g., the function checking for the presence of a clique in a graph and the determinant of a boolean matrix.

2. Quantum Branching Programs

In this section, we define classical and quantum variants of branching programs and discuss basic properties of the quantum variant. An extensive survey of results for classical branching programs is given in the monograph of Wegener [42].

Definition 2.1: A (*deterministic*) *branching program (BP)* on the variable set $X = \{x_1, \dots, x_n\}$ is a directed acyclic graph with a designated *start node* and two sinks. The sinks are labeled by the constants 0 and 1, resp. Each interior node is labeled by a variable from X and has two outgoing edges carrying labels 0 and 1, resp. This graph computes a boolean function f defined on X as follows. To compute $f(a)$ for some input $a = (a_1, \dots, a_n) \in \{0, 1\}^n$, start at the start node. For an interior node labeled by x_i , follow the edge labeled by a_i (this is called *testing* the variable). Iterate this until a sink is reached, whose label gives the value $f(a)$. For a fixed input a , the sequence of nodes visited in this way is called the *computation path for a*. The *size* $|G|$ of a branching program is the number of its nodes. Its *width* is the maximum number of nodes with the same distance from the start node. The *branching program size* of a function f is the minimum size of a branching program that computes it.

BPs are a nonuniform model of computation, so we usually consider a sequence $(G_n)_{n \in \mathbb{N}}$ of BPs representing a sequence of boolean functions $(f_n)_{n \in \mathbb{N}}$, where G_n represents the function $f_n: \{0, 1\}^n \rightarrow \{0, 1\}$. We will encounter the following variants of BPs.

Definition 2.2:

- A BP is called *read-once* if, for each variable x_i , each of the paths in the BP contains at most one node labeled by x_i .
- A BP is called *leveled* if the set of its nodes can be partitioned into disjoint sets V_1, \dots, V_ℓ , where V_i is called the *i th level*, such that for $1 \leq i \leq \ell - 1$, each edge leaving a node in V_i reaches a node in V_{i+1} .
- An *OBDD* (ordered binary decision diagram) is a read-once BP where on each computation path the variables are tested according to the same order. For the variable order π it is also called π -OBDD.

Definition 2.3: A *randomized BP* is defined as a deterministic BP, but may additionally contain unlabeled *randomized nodes* with two unlabeled outgoing edges, may contain cycles, and may have sinks labeled by 0, 1, or “?”. The computation for an input a is carried out by starting at the start node, following the outgoing edge labeled by a_i for an x_i -node as for deterministic BPs, and taking one of the outgoing edges with probability 1/2 for randomized nodes until a sink is reached, where different randomized decisions are independent of each other. The probability that the randomized BP computes the output $r \in \{0, 1, ?\}$ for the input a is the probability that the computation for a reaches a sink labeled by r .

Different modes of acceptance with unbounded, bounded (two-sided), one-sided, and zero error are defined as usual (see, e. g., [32, 42]). Randomized variants of the restricted models of BPs from Definition 2.2 are obtained by applying the respective restriction to the nodes labeled by variables.

Next, we define a quantum variant of BPs. This definition contains the alternative definitions in the literature as special cases.

Definition 2.4: A *quantum branching program (QBP)* over the variable set $X = \{x_1, \dots, x_n\}$ is a directed multigraph $G = (V, E)$ with a *start node* $s \in V$, a set $F \subseteq V$ of sinks, and (*transition amplitudes*) $\delta: V \times V \times \{0, 1\} \rightarrow \mathbb{C}$. Each node $v \in V - F$ is labeled by a variable $x_i \in X$ and we define $\text{var}(v) = i$. Each node $v \in F$ carries a label from $\{0, 1, ?\}$, denoted by $\text{label}(v)$. Each edge $(v, w) \in E$ is labeled by a boolean constant $b \in \{0, 1\}$ and the amplitude $\delta(v, w, b)$. An edge with boolean label b is called *b -edge* for short. We assume that there is at most one edge carrying the same boolean label between a pair of nodes and set $\delta(v, w, b) = 0$ for all $(v, w) \notin E$ and $b \in \{0, 1\}$.

The graph G is required to satisfy the following two constraints. First, it has to be *well-formed*, meaning that for each pair of nodes $u, v \in V - F$ and all assignments $a = (a_1, \dots, a_n)$ to the variables in X ,

$$\sum_{w \in V} \delta^*(u, w, a_{\text{var}(u)}) \delta(v, w, a_{\text{var}(v)}) = \begin{cases} 1, & \text{if } u = v; \text{ and} \\ 0, & \text{otherwise.} \end{cases} \quad (\text{W})$$

Second, G has to be *unidirectional*, which means that for each $w \in V$, all nodes $v \in V$ such that $\delta(v, w, b) \neq 0$ for some $b \in \{0, 1\}$ are labeled by the same variable.

The well-formedness constraint implies that the QBP has a unitary time evolution operator (see below) and is, therefore, motivated by the laws of quantum theory. Unidirectionality is a property that makes understanding and manipulating models of quantum computation much easier. We discuss this issue in more detail in Section 3. Since unidirectionality is crucial for our simulations, we include this requirement in the definitions of QBPs. Next, we define the semantics of QBPs.

Definition 2.5 (Computation of a QBP): Let $G = (V, E)$ be a QBP on n variables with start node $s \in V$, sinks $F \subseteq V$, and transition amplitudes δ . Let $\mathcal{H} = \mathbb{C}^{|V|}$ and let $(|v\rangle)_{v \in V}$ be an orthonormal basis of \mathcal{H} . Let $a = (a_1, \dots, a_n)$ be an assignment to the variables of G . Let $L(a)$ be the linear transformation from the subspace spanned by all $|v\rangle$, $v \in V - F$, into \mathcal{H} such that for $v \in V - F$,

$$L(a)|v\rangle = \sum_{w \in V} \delta(v, w, a_{\text{var}(v)})|w\rangle.$$

Due to the well-formedness constraint (W), $L(a)$ can be extended to a unitary transformation $U(a)$ on \mathcal{H} . Call $U(a)$ a *time evolution operator* of the QBP for input a . Define projection operators on \mathcal{H} by setting

$$E_{\text{cont}} = \sum_{v \in V - F} |v\rangle\langle v|, \quad E_{\text{stop}} = \sum_{v \in F} |v\rangle\langle v|, \quad \text{and} \quad E_r = \sum_{v \in V, \text{label}(v)=r} |v\rangle\langle v|, \quad \text{for } r \in \{0, 1, ?\}.$$

For $T \in \mathbb{N}_0$ and $r \in \{0, 1, ?\}$ define

$$p_{G,r}(a, T) = \sum_{t=0}^T \|E_r(U(a)E_{\text{cont}})^t|s\rangle\|^2 \quad \text{and} \quad p_{G,r}(a) = p_{G,r}(a, \infty),$$

the *probability that G outputs r for input a during the first T time steps* and the (*absolute*) *probability that G outputs r for input a* , resp.

QBPs computing a function $f: \{0, 1\}^n \rightarrow \{0, 1\}$ with *unbounded error*, *bounded (two-sided) error*, and *one-sided error* are defined in the straightforward way. We say that G computes f with *zero error and failure probability* ε , $0 \leq \varepsilon < 1$, if $p_{G, \neg f(a)}(a) = 0$ and $p_{G, ?}(a) \leq \varepsilon$ for all $a \in \{0, 1\}^n$. We say that G *computes f exactly* if it computes f with zero error and failure probability 0.

Let the (*worst-case*) *running time of G on a* be

$$T_G(a) = \min\{T \mid T \in \mathbb{N}_0 \cup \{\infty\}, p_{G,0}(a, T) + p_{G,1}(a, T) + p_{G,?}(a, T) = 1\}.$$

The running time can be in \mathbb{N}_0 , infinite, or undefined. The *expected running time of G on a* is defined by

$$\bar{T}_G(a) = \sum_{t=0}^{\infty} t \cdot \|E_{\text{stop}}(U(a)E_{\text{cont}})^t|s\rangle\|^2.$$

We say that G *runs in time T* if $T_G(a) \leq T$ for all $a \in \{0, 1\}^n$. Furthermore, G *runs in expected time T* if $\bar{T}_G(a) \leq T$ for all $a \in \{0, 1\}^n$.

Since the QBP does not have edges leaving the sinks, the time evolution operator is merely an extension of the mapping $L(a)$ and, therefore, not necessarily uniquely determined.

In the remainder of this section we discuss the relationship between (classical) BPs and QBPs, and some variants of the definition of QBPs. Because of the well-formedness and the unidirectionality requirements of QBPs it is not obvious whether functions with small size BPs also have small size QBPs. In order to prove such a statement, we introduce the notion of reversibility.

Definition 2.6: A BP is *reversible* if each node is reachable from at most one node v by a 0-edge and from at most one node w by a 1-edge and v and w are labeled by the same variable.

Reversible BPs are obviously special QBPs. Furthermore, as proved by Špalek [37] using a similar construction of Lange, McKenzie, and Tapp [23] for Turing machines, any (possibly non-reversible) BP of size $s(n) = \Omega(n)$ can efficiently be simulated by a reversible one of size $\text{poly}(s(n))$. This implies:

Proposition 2.7 ([37]): *If the sequence of functions $(f_n)_{n \in \mathbb{N}}$ has BPs $(G_n)_{n \in \mathbb{N}}$ of size $s(n) = \Omega(n)$, it also has QBPs $(G'_n)_{n \in \mathbb{N}}$ of size $\text{poly}(s(n))$.*

Adleman, DeMarras, and Huang [3] have shown that uniform QTMs with arbitrary complex amplitudes can decide certain languages of arbitrarily high Turing degree in polynomial time and are thus too powerful to be realistic. For randomized classical as well as quantum models of computation, practical considerations (depending on the details of the physical implementation of the model) lead to restrictions on the set of allowed amplitudes. However it is not obvious what a natural restriction in the nonuniform, space-bounded scenario is. The following definition is motivated by the goal of finding the least restrictive definition that still allows the resulting QBPs to be simulated efficiently by the corresponding standard QTM model. Recall that an *algebraic number (over \mathbb{Q})* is an $x \in \mathbb{C}$ such that there is a rational polynomial with root x .

Definition 2.8: A sequence $(G_n)_{n \in \mathbb{N}}$ of QBPs has *short amplitudes* if for some number k independent from the input length there are algebraic numbers $\alpha_1, \dots, \alpha_k$, such that each amplitude of each G_n can be written as $p(\alpha_1, \dots, \alpha_k)$ for some k -variate rational polynomial p of degree $\text{poly}(|G_n|)$ whose coefficients are fractions with numerator and denominator each of bit length at most $\text{poly}(|G_n|)$.

The requirements of this definition are obviously satisfied in the special case that the sequence of QBPs uses only amplitudes from a fixed, finite set of algebraic numbers. This is the situation investigated for uniform, space-restricted QTMs by Watrous [40, 41]. Among other results, we show in Section 4 that unidirectional nonuniform QTMs with algebraic amplitudes and QBPs with short amplitudes are equivalent in computational power under space restrictions, which serves as a motivation for the above definition.

We conclude the discussion on reasonable restrictions for the amplitudes with some simple observations. First, QBPs with complex amplitudes can be transformed into equivalent QBPs with real amplitudes, where the number of nodes increases by a factor of at most 2 (cf. Proposition 5.3 in [41]). The main idea is to replace each node v with two nodes v_r and v_i such that the corresponding vectors $|v_r\rangle$ and $|v_i\rangle$ carry the real and imaginary part of the amplitude of $|v\rangle$, resp. Second, in Definition 2.8 the number k of algebraic numbers can be replaced with 1, since by the primitive element theorem from algebra, the algebraic numbers $\alpha_1, \dots, \alpha_k$ can be represented as polynomials in a single algebraic number α . Since k as well as $\alpha_1, \dots, \alpha_k$ are independent from the input size, these polynomials have a constant number of constant coefficients such that the resulting QBP still has short amplitudes. Finally, since the bit lengths of the denominators of all coefficients are bounded by $\text{poly}(|G_n|)$ and the numbers of edges and, therefore, the number of denominators is bounded by $2|G_n|^2$, all the coefficients have a common denominator m of bit length $\text{poly}(|G_n|)$. We obtain the following result.

Proposition 2.9: *Each sequence $(G_n)_{n \in \mathbb{N}}$ of QBPs with short amplitudes can be simulated by a sequence $(G'_n)_{n \in \mathbb{N}}$ of QBPs with $|G'_n| \leq 2|G_n|$ such that there is a single algebraic number α and a number $m = 2^{\text{poly}(|G'_n|)}$ such that each amplitude of G'_n can be written as $p(\alpha)/m$ for an integer polynomial p with a degree bounded by $\text{poly}(|G'_n|)$ and coefficients bounded above in absolute value by $2^{\text{poly}(|G'_n|)}$.*

As for classical BPs, it is possible to simplify the structure of QBPs without increasing their size too much. The following has been observed by Špalek [37].

Proposition 2.10 ([37]): *Let G be a QBP and let $t \in \mathbb{N}_0$. Then there is a leveled QBP G' with $t + 1$ levels that for each input a computes an output $r \in \{0, 1, ?\}$ with probability $p_{G,r}(a, t)$ after carrying out exactly t computation steps and that does not stop before. The size of G' is bounded above by $(t + 1)^2|G|$.*

For the construction of QBPs, it is convenient to allow *unlabeled nodes* with an arbitrary number of outgoing edges carrying only amplitude labels. An unlabeled node v can be understood as an abbreviation for a node that is labeled by some input variable, where the value of this variable does not influence the computation. This means that each edge leading from the unlabeled node v to w has to be replaced with a 0-edge and a 1-edge from v to w which both have the same amplitude label as the original edge from v to w . When using unlabeled nodes we have to make sure that the QBP resulting from this transformation is unidirectional and well-formed.

3. Definitions and Tools for Quantum Turing Machines

We first introduce a nonuniform variant of quantum Turing machines (QTMs). The definition is similar to those of Bernstein and Vazirani [11] and Nishimura and Ozawa [27] for the uniform setting. Afterwards, we collect tools for approximately performing arbitrary unitary transformations by QTMs.

Definition 3.1: A *nonuniform (or advice-taking) quantum Turing machine* is a QTM $M = (Q, \Sigma, \delta)$ together with an advice function $\text{adv}: \mathbb{N} \rightarrow \Sigma^*$, where Q is a finite set containing q_0, q_f and $\Sigma = \Sigma_1 \times \dots \times \Sigma_k$ with finite sets $\Sigma_1, \dots, \Sigma_k$ each containing $\{0, 1, ?, B\}$. The QTM M has the initial state q_0 and the unique final state q_f , and “ B ” is used as the blank symbol. The machine is equipped with three tapes, a read-only input tape, a read-only advice tape, and the work tape. All tapes are two-way infinite and indexed by \mathbb{Z} and each is split into k separate tracks that may contain symbols from $\Sigma_1, \dots, \Sigma_k$. We have $\delta: (Q \times \Sigma^3) \times (Q \times \Sigma \times \{-1, 0, 1\}^3) \rightarrow \mathbb{C}$, and $\delta((q, \sigma_i, \sigma_a, \sigma_w), (q', \sigma'_w, d_i, d_a, d_w))$ is the amplitude for a transition from state q , with symbols $\sigma_i, \sigma_a, \sigma_w$ on the input, advice, and work tape, resp., to state q' , writing σ'_w on the work tape and moving the heads on the three tapes according to d_i, d_a, d_w . Upon start of the machine, the input tape is loaded with the input string $x \in \{0, 1\}^*$ at positions $0, \dots, |x| - 1$ of the first track. The advice tape is loaded with the advice string $\text{adv}(|x|) \in \Sigma^*$ at positions $0, \dots, |\text{adv}(|x|)| - 1$. All other tape positions contain blanks, all heads are at position 0 and the finite control of M is in its initial state. A *configuration* of M is a tuple (q, w, i, j, k) , with the current state of the finite control $q \in Q$, the contents $w \in \Sigma^*$ of the work tape, and the positions $i, j, k \in \mathbb{Z}$ of the heads on the input, advice, and work tape, resp. Let $\mathcal{C}_n(M)$ be the set of all configurations of M for inputs of length n . Let $\mathcal{H} = \mathbb{C}^{|\mathcal{C}_n(M)|}$ be the Hilbert space spanned by all configurations from $\mathcal{C}_n(M)$, which we identify with vectors from an orthonormal basis. The *time evolution operator* $U(a)$ describes the application of the transition function δ to a superposition of configurations, where the input is a . The *well-formedness constraint* requires $U(a)$ to be unitary for all inputs a .

Definition 3.2 (Computation of a nonuniform QTM): Let $M = (Q, \Sigma, \delta)$ be as in the above definition. A QTM indicates stopping by entering q_f and signals its output by an entry at position 0, called the *output cell*, of a designated track of the work tape, called the *output track*. Define $E_{\text{state}}(A)$ as the projection operator over \mathcal{H} onto the subspace spanned by all configurations with state in $A \subseteq Q$. Then the projections $E_{\text{state}}(\{q_f\}), E_{\text{state}}(Q - \{q_f\})$ describe

the measurement checking whether the current state is equal to q_f . This measurement is performed before each computation step. If the QTM does not stop, $U(a)$ is applied to the state after the measurement. Let $E_{\text{result}}(r)$, $r \in \{0, 1, ?\}$, be the projection onto the subspace spanned by the configurations with result r in the output cell. If stopping of the QTM has been detected, the measurement described by these latter projections is carried out in order to determine the result of the computation. For $T \in \mathbb{N}_0$ and $r \in \{0, 1, ?\}$, let

$$p_{M,r}(a, T) = \sum_{t=0}^T \left\| E_{\text{result}}(r) E_{\text{state}}(\{q_f\}) (U(a) E_{\text{state}}(Q - \{q_f\}))^t |s\rangle \right\|^2$$

be the *probability that M outputs r on input a during the first T computation steps*. Based on these probabilities, acceptance of the QTM with different types of error is defined as usual. The (*expected*) *running time of M on a* , denoted by $T_M(a)$ ($\overline{T}_M(a)$), is defined analogously to QBPs (Definition 2.5). The *space used by M on input $a \in \{0, 1\}^*$* is the maximum number of cells on the work tape between the leftmost and rightmost non-blank symbol taken over all configurations which are reached with nonzero amplitude during the computation on input a and in which the machine has not yet halted. The (*total*) *space $s_M(a)$ used by M on input $a \in \{0, 1\}^*$* is defined as the sum of the space on the work tape and $\lceil \log |\text{adv}(|a|)| \rceil$. Finally, we say that *M runs in space $s: \mathbb{N} \rightarrow \mathbb{N}_0$* if for all $a \in \{0, 1\}^n$, $s_M(a) \leq s(n)$.

Definition 3.3: A *reversible Turing machine (RTM)* is a deterministic TM where each configuration has at most one predecessor. A TM or QTM M is called *unidirectional* if each state can be entered from only one direction on each tape, i. e., if there are functions $D_i, D_a, D_w: Q \rightarrow \{-1, 0, 1\}$ such that $\delta((q, \sigma_i, \sigma_a, \sigma_w), (q', \sigma'_i, d_i, d_a, d_w)) \neq 0$ only if $D_i(q') = d_i$, $D_a(q') = d_a$ and $D_w(q') = d_w$.

Unidirectionality is a crucial property of QTMs that makes working with them much easier. The property has first been investigated by Bernstein and Vazirani [11] for single-tape QTMs that are additionally *two-way*, i. e., are required to move their head in each computation step. Their results include that single-tape RTMs (even with stationary tape heads allowed) are automatically unidirectional and, furthermore, that single-tape two-way QTMs can be simulated time and space efficiently by unidirectional ones. Furthermore, it is well known that also QTMs with stationary tape heads allowed can be time efficiently simulated by unidirectional ones using the simulations of QTMs by quantum circuits and vice versa due to Yao [43] and Nishimura and Ozawa [27]. These results cannot be applied in an obvious way in the space-bounded scenario. Already for TMs with only one additional input tape, reversibility does no longer imply unidirectionality, as simple examples show. In Section 5 we show that general nonuniform QTMs with sublinear space can be space efficiently simulated by unidirectional ones.

For constructing unidirectional nonuniform QTMs, we need the usual toolbox of programming primitives that allows us to work with multiple tracks, combine TMs, construct looping TMs and so on. We use appropriate versions of lemmas for these tasks due to Bernstein and Vazirani [11]. We only remark that, by going through their proofs, it is straightforward to extend these lemmas to unidirectional RTMs and unidirectional QTMs, resp., with an arbitrary number of read-only input tapes. This includes nonuniform machines as a special case.

In simulations of other models of quantum computation by QTMs, we face the problem of carrying out an arbitrary given unitary transformation over a finite-dimensional Hilbert space using only a finite program for the QTM. For doing this, we use a result due to Harrow, Recht, and Chuang [14] that allows us to approximate any unitary operator over a finite-dimensional Hilbert space by a product of “few” elements from a finite collection of “simple”

unitary transformations. The approximation is with respect to the *operator norm*, defined for an operator A over a Hilbert space \mathcal{H} by $\|A\| = \sup\{\|Ax\| \mid x \in \mathcal{H}, \|x\| \leq 1\}$. We say that A' is an ε -*approximation of A* or *approximates A with error ε* if $\|A' - A\| \leq \varepsilon$.

Define the unitary matrices

$$V_1 = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2\sqrt{-1} \\ 2\sqrt{-1} & 1 \end{pmatrix}, V_2 = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2 \\ -2 & 1 \end{pmatrix}, \text{ and } V_3 = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 + 2\sqrt{-1} & 0 \\ 0 & 1 - 2\sqrt{-1} \end{pmatrix}.$$

For $i \in \{1, 2, 3\}$ let $V_{i+3} = V_i^{-1}$. Let $\mathcal{G}_2 = \{V_1, \dots, V_6\}$. For $i \in \{1, \dots, 6\}$ and $j \in \{1, \dots, d-1\}$ define the unitary $d \times d$ -matrix $W_{i,j}$ by setting

$$W_{i,j}|k\rangle = \begin{cases} (V_i)_{1,1}|j\rangle + (V_i)_{2,1}|j+1\rangle, & \text{if } k = j; \\ (V_i)_{1,2}|j\rangle + (V_i)_{2,2}|j+1\rangle, & \text{if } k = j+1; \\ |k\rangle, & \text{otherwise.} \end{cases}$$

Let \mathcal{G}_d be the set of all $W_{i,j}$ with $i \in \{1, \dots, 6\}$ and $j \in \{1, \dots, d-1\}$. Recall that $\text{SU}(d)$ denotes the set of all unitary $d \times d$ -matrices. Harrow, Recht, and Chuang [14] have proved the following lemma, where we have added the estimate of the bound for k depending on d , while in [14] the dimension is regarded as a constant.

Lemma 3.4 ([14]): *There is a constant $c > 0$ such that for all $\varepsilon > 0$, $U \in \text{SU}(d)$, and $k = \lceil cd^2 \log(d/\varepsilon) \rceil$, there are $U_1, \dots, U_k \in \mathcal{G}_d$ such that $\|U - U_1 \cdots U_k\| \leq \varepsilon$.*

Call the matrices $W_{i,j}$ with $i \in \{1, \dots, 6\}$ and $j \in \{1, \dots, d-1\}$ *elementary*. Let $d = 2^m$ and let $|\psi\rangle \in \mathbb{C}^d$ be encoded in $m = \log d$ qubits on the work tape of a QTM. Given i, j as additional inputs, we would like to compute $W_{i,j}|\psi\rangle$, as required for the application of Lemma 3.4. Bernstein and Vazirani [11] have shown how to implement this for a different set of two-dimensional transformations. By an easy adaptation of their construction and an application of the simulation of single-tape two-way QTMs by unidirectional ones also from their paper, we obtain:

Lemma 3.5 ([11]): *There is a unidirectional single-tape QTM M_{elem} with multiple tracks that works as follows. Let $d = 2^m$ and let $|\psi\rangle \in \mathbb{C}^d$ be a superposition of m qubits. Let $c(i, j)$ consist of the binary codes of $i \in \{1, \dots, 6\}$ and $j \in \{1, \dots, d-1\}$. Started with $|\psi\rangle$ in tape cells $0, \dots, m-1$ of the first track and $|c(i, j)\rangle$ in the tape cells $0, \dots, |c(i, j)|-1$ of the second track, M_{elem} computes the output $W_{i,j}|\psi\rangle$ on the first track, replacing $|\psi\rangle$, in time and space $O(m)$. Furthermore, the running time of M_{elem} only depends on m , the length of the contents on the first track.*

Combining Lemmas 3.4 and 3.5, we can use a QTM to compute a good approximation of any desired finite-dimensional unitary transformation. We still have to make sure that measuring the state after applying the approximate transformation gives a result that agrees with that after applying the original transformation with high probability. This can be shown using the following statements. The first one is due to Bernstein and Vazirani [11], the proof of second one is analogous to that of a similar statement in [26], page 195.

Proposition 3.6: *Let U, U_1, \dots, U_n , and V_1, \dots, V_n be operators over a Hilbert space \mathcal{H} with $\|U_i\|, \|V_i\| \leq 1$ and $\|U_i - V_i\| \leq \varepsilon_i$ for $i = 1, \dots, n$. Then $\|U_1 \cdots U_n - V_1 \cdots V_n\| \leq \varepsilon_1 + \cdots + \varepsilon_n$.*

Lemma 3.7: *Let $\varepsilon > 0$ and $t \in \mathbb{N}$. Let U and U' be unitary operators over a Hilbert space \mathcal{H} with $\|U - U'\| \leq \varepsilon$. Let P, Q be projections over \mathcal{H} . Let $|v\rangle \in \mathcal{H}$ with $\|v\rangle\| = 1$. Define $p = \|Q(UP)^t|v\rangle\|^2$ and $p' = \|Q(U'P)^t|v\rangle\|^2$. Then $|p - p'| \leq 2t\varepsilon$.*

4. Equivalence of QBPs and Space-Bounded Unidirectional Nonuniform QTMs

We prove our simulation results for QBPs and unidirectional nonuniform QTMs. We first provide a basic theorem that allows a step-by-step simulation of unidirectional nonuniform QTMs by QBPs and vice versa. Each step of a QBP can only be done approximately by a unidirectional nonuniform QTM. In order to control the total error, we have to specify the number of simulation steps in advance. This raises the problem of bounding the computation time of space-bounded algorithms that is studied afterwards. We first define a suitable notion of simulations.

Definition 4.1: Let M_1, M_2 be nonuniform QTMs or QBPs. As defined in Sections 2 and 3, let $p_{M_i, r}(a, T)$ be the probability that M_i computes the output r on the input a during the first T computation steps. We say that M_1 *simulates* T steps of M_2 in T' steps with accuracy $\varepsilon \geq 0$, if for all $a \in \{0, 1\}^*$ and $r \in \{0, 1, ?\}$: $|p_{M_1, r}(a, T') - p_{M_2, r}(a, T)| \leq \varepsilon$. We say that M_1 *simulates* M_2 if M_1 simulates T steps of M_2 in the same number of steps with accuracy $\varepsilon = 0$ for arbitrary T .

4.1. Basic Step-by-Step Simulations

Theorem 4.2:

- (i) Let M be a unidirectional nonuniform QTM that runs in space $S(n) = \Omega(\log n)$. Then there is a sequence of QBPs $(G_n)_{n \in \mathbb{N}}$ with $|G_n| = 2^{O(S(n))}$ that simulate M .
- (ii) Let $(G_n)_{n \in \mathbb{N}}$ be a sequence of QBPs with $|G_n| = \Omega(n)$. Let $\varepsilon: \mathbb{N} \rightarrow (0, 1)$ and $T: \mathbb{N} \rightarrow \mathbb{N}_0$. Then there is a unidirectional nonuniform QTM that for each $n \in \mathbb{N}$ simulates $T(n)$ steps of G_n in $\text{poly}(|G_n|, T(n), \log(1/\varepsilon(n)))$ steps with accuracy $\varepsilon(n)$ and runs in space $O(\log |G_n| + \log \log(T(n)/\varepsilon(n)))$.

We discuss the consequences of this theorem for the motivation of our QBP model and the relationship between QBPs and QTMs in detail in Section 4.2.

Proof of Theorem 4.2, Part (i). This follows by an easy adaptation of the proof of the analogous result for classical BPs and TMs. Let $M = (Q, \Sigma, \delta)$ be a unidirectional nonuniform QTM with advice function $\text{adv}: \mathbb{N} \rightarrow \Sigma^*$ that runs in space $S(n) = \Omega(\log n)$. We ensure that the heads on the input and advice tape stay in the area consisting of the non-blank cells (see [38] for details). Then M has at most $2^{O(S(n))}$ configurations.

We construct the QBP G over the variable set $X = \{x_0, \dots, x_{n-1}\}$ with $\mathcal{C}_n(M)$ as its node set. For a configuration $c \in \mathcal{C}_n(M)$ of M where the head on the input tape is at position $i \in \{0, \dots, n-1\}$, define $\text{var}(c) = i$ in G (recall that $\text{var}(c)$ denotes the index of the variable with which a QBP node is labeled). For an input with bit $b \in \{0, 1\}$ at position i on the input tape of M , let the application of the transition function δ of M to $|c\rangle$ yield the superposition

$$\sum_{c' \in \mathcal{C}_n(M)} \alpha(c, c', b) |c'\rangle, \quad \alpha(c, c', b) \in \mathbb{C}.$$

For each $\alpha(c, c', b) \neq 0$, we add a b -edge from c to c' in G and use $\alpha(c, c', b)$ as the amplitude label of this edge. We define the start node of G as the initial configuration of M and identify the set of final nodes F with the set of final configurations of M .

The graph G defined above fulfills the well-formedness requirement of QBPs since the time evolution operator of the QTM M is unitary. In order to prove that G is unidirectional assume for a contradiction that the node v has predecessors v_1 and v_2 labeled by different variables. Then during the transitions of M that correspond to the transition of v_1 to v and v_2 to v the head on the input tape makes different moves in contradiction to the unidirectionality of M . Since $|\mathcal{C}_n(M)| = 2^{O(S(n))}$, the branching program is of the required size. It is easy to verify that G simulates M because of the similarity of the definitions of the semantics for the two models. \square

Proof of Theorem 4.2, Part (ii). Let G be the QBP to be simulated and let $X = \{x_0, \dots, x_{n-1}\}$ be the variable set of G . In a first step, we show how to transform G into an equivalent QBP G' which has the additional property that all nodes that are reachable from the start node by a path of length t are labeled by $x_{t \bmod n}$. This allows us to decompose the time evolution operator into n factors where each factor only depends on the value of one of the variables. In a second step we construct a nonuniform QTM and its advice string from the decomposed time evolution operator of G' and prove the claims on the resources required by this QTM.

Let $G = (V, E)$ and let s and F denote the start node and the set of sinks of G , resp. Due to the unidirectionality of G , all predecessors of a node $v \in V$ are labeled by the same variable, whose index is denoted by $\text{pre}(v)$. If the start node does not have any predecessor, let $\text{pre}(s) = n - 1$. Furthermore, we set $\text{var}(v) = 0$ for $v \in F$.

We construct the QBP $G' = (V', E')$ from G by adding dummy nodes. Let $V' = \{(v, i) \mid v \in V, i \in \{\text{pre}(v) + 1, \dots, n - 1, 0, \dots, \text{var}(v)\}\}$. Let $s' = (s, 0)$ be the start node of G' and let $F' = \{(v, 0) \mid v \in F\}$ be its set of sinks. Define $\text{var}(v, i) = i$ for all $v \in V$ and $\text{label}(v, 0) = \text{label}(v)$ for all $v \in F$. For each $(v, w) \in E$, add an edge $((v, \text{var}(v)), (w, (\text{pre}(w) + 1) \bmod n))$ to E' that inherits all labels of the edge (v, w) . Furthermore, for each $w \in V$, $i \in \{\text{pre}(w) + 1, \dots, n - 1, 0, \dots, \text{var}(w) - 1\}$, and $b \in \{0, 1\}$, add an edge $((w, i), (w, (i + 1) \bmod n))$ to E' with boolean label b and amplitude 1. Let δ' be the transition amplitudes of G' defined in this way. It is easy to see that G' is a QBP. Well-formedness and unidirectionality of G' follow from the respective properties of G for the subgraph induced by the nodes in $\{(v, \text{var}(v)), (v, (\text{pre}(v) + 1) \bmod n) \mid v \in V\}$ and are obvious for the rest of the graph. It is easy to see that $|G'| = O(n|G|)$.

Claim. G' simulates T steps of G in nT steps with accuracy 0. Furthermore, there are unitary operators $U_i(b)$ with $0 \leq i \leq n - 1$ and $b \in \{0, 1\}$ such that for any time evolution operator $U'(a)$ of G' with $a \in \{0, 1\}^n$, the projection E'_{cont} to the space spanned by the non-sink nodes of G' , the start node s' of G' , and any $T \in \mathbb{N}_0$, $(U'(a)E'_{\text{cont}})^{nT}|s'\rangle = ((U_{n-1}(a_{n-1}) \cdots U_0(a_0))E'_{\text{cont}})^T|s'\rangle$.

Proof of the claim. For the proof that G' simulates T steps of G with nT of its own steps, let φ be the linear embedding of the superpositions of G into those of G' induced by setting $\varphi(|v\rangle) = |(v, 0)\rangle$ for $v \in V$. Let $U(a)$ and $U'(a)$ be time evolution operators of G and G' , resp., for the input $a \in \{0, 1\}^n$. Let E_{cont} , E_r and E'_{cont} , E'_r be the projections to the spaces spanned by the non-sink nodes and nodes with output label r , resp., for the graphs G and G' , resp. An easy induction shows that for each $T \in \mathbb{N}_0$, $(U'(a)E'_{\text{cont}})^{nT}|s'\rangle = \varphi((U(a)E_{\text{cont}})^T|s\rangle)$. Furthermore, $E'_r\varphi(|v\rangle) = \varphi(E_r|v\rangle)$ for all $v \in V$. Hence, $p_{G',r}(a, nT) = p_{G,r}(a, T)$ for all $T \in \mathbb{N}_0$ and G' simulates T steps of G with nT steps.

Furthermore, it is also easy to prove by induction that for any $T \in \mathbb{N}_0$, $i = T \bmod n$, and any $v \in V' - F'$ with $\text{var}(v) \neq i$, $\langle v|E'_{\text{cont}}(U'(a)E'_{\text{cont}})^T|s'\rangle = \langle v|(U'(a)E'_{\text{cont}})^T|s'\rangle = 0$. Hence, instead of applying $U'(a)$ in the $(T + 1)$ -st computation step, we may apply a unitary extension $U_i(a_i)$ of the mapping defined by $|v\rangle \mapsto \sum_{w \in V'} \delta'(v, w, a_i)|w\rangle$ for $v \in V'$ with $\text{var}(v) = i$,

without changing the computed superposition. Finally, for all $v \in F'$ and $T \bmod n \neq 0$, we have $\langle v | (U'(a)E'_{\text{cont}})^T | s' \rangle = 0$. By induction, it follows that for any $T \in \mathbb{N}_0$, $(U'(a)E'_{\text{cont}})^{nT} | s' \rangle = ((U_{n-1}(a_{n-1}) \cdots U_0(a_0))E'_{\text{cont}})^T | s' \rangle$, as claimed. \square

Now we describe the second step of the proof, the construction of the QTM from G' . Let $s = O(n|G|)$ be the number of nodes of G' . Let $m = \lceil \log s \rceil$. It is convenient to assume that the node numbers have the length $m + 2$, where the numbers of interior nodes begin with 00 and the numbers of 0- and 1-sinks with 01 and 11, resp. Furthermore, we assume that the start node has the number 0.

Construction of the advice string. First, we define approximate representations for each matrix $U_i(b)$, $0 \leq i \leq n - 1$ and $b \in \{0, 1\}$, as a list of elementary matrices using Lemma 3.4. Choosing $\varepsilon' = \varepsilon/(2nT^2)$ as the error bound and s as the dimension of the Hilbert space, Lemma 3.4 yields $s \times s$ -matrices $U_{i,0}(b), \dots, U_{i,k-1}(b)$ whose product is an ε' -approximation of $U_i(b)$, where $k = O(s^2 \log(s/\varepsilon')) = O(s^2 \log(nsT/\varepsilon))$ is the number of matrices obtained from the lemma. Observe that the number of elementary matrices in the representation of $U_i(b)$ is the same for all i and b . Elementary matrices are encoded such that the corresponding unitary transformations can be applied using the QTM provided in Lemma 3.5. The code for an elementary matrix $W_{j,j'}$ consists of the binary codes of $j \in \{1, \dots, 6\}$ and $j' \in \{1, \dots, s - 1\}$.

On the advice tape, we store the codes of the elementary matrices $U_{i,\ell}(b)$ for $0 \leq i \leq n - 1$, $b \in \{0, 1\}$, and $\ell \in \{0, \dots, k - 1\}$, as well as some additional administrative information. The information is organized using four tracks, where the non-blank part of each track starts at position 0:

Track 1: Binary code of the input length n .

Track 2: Binary code of k .

Track 3: Binary code of the length of the code for an elementary matrix.

Track 4: List of codes for all $U_{i,\ell}(b)$.

The length of the code of each elementary matrix is $O(\log s)$. Each of the $2n$ matrices $U_i(0)$ and $U_i(1)$ is encoded using $O(k \log s)$ bits. We have $k = O(s^2 \log(nsT/\varepsilon))$. Hence, the length of the information on track 4 is bounded by $O(2n \cdot k \log s) = \text{poly}(s, \log(T/\varepsilon))$, which is also a bound on the overall length of the advice string. The logarithm of this, $O(\log s + \log \log(T/\varepsilon)) = O(\log |G| + \log \log(T/\varepsilon))$, is the contribution of the advice tape to the space.

Construction of the QTM. The QTM uses the following tracks on the work tape:

Track 1: Output track. The output of the QTM is in cell 0 of this track upon termination.

Track 2: Node register consisting of $m + 2$ cells that contains the current superposition of node numbers of G' .

Track 3: Buffer for the code of $U_{i,\ell}(x_i)$.

Track 4: Counter i with values in $\{0, \dots, n - 1\}$.

Track 5: Counter ℓ with values in $\{0, \dots, k - 1\}$.

Track 6: Buffer for the value of the current input bit.

Track 7: Buffer for the position of the currently applied $U_{i,\ell}(x_i)$ on the advice tape.

Initially, the work tape only contains blanks. By choosing an appropriate encoding of binary numbers (see, e. g., [39]), we ensure that a string of blanks represents the number 0. Hence, the counters on track 4 and track 5 are initialized with 0. Since the start node has the number 0, the blanks from the initialization of the node register encode the start node.

1. Forever do
2. *Termination check.* Swap the contents of cell 0 of the node register (signaling the output if the current node is a sink) and the output cell. If cell 1 of the node register contains a 1 (signaling a sink), enter q_f . Otherwise, swap again the contents of cell 0 of the node register and the output cell.
3. For $i := 0$ to $n - 1$ do
4. XOR track 6 with the value of x_i .
5. For $\ell := 0$ to $k - 1$ do
6. XOR track 7 with the position of the code of $U_{i,\ell}(x_i)$ on the advice tape.
7. XOR track 3 with the code of $U_{i,\ell}(x_i)$ from the advice tape.
8. Apply $U_{i,\ell}(x_i)$ to the node register.
9. Repeat step 7; this erases track 3.
10. Repeat step 6; this erases track 7.
11. Repeat step 4; this erases track 6.

Figure 2: Algorithm for the nonuniform QTM simulating G' .

The algorithm performed by the QTM is shown in Figure 2. The algorithm consists of an infinite loop whose body, steps 2–11, simulates one computation step of the QBP G' . The loop is left and the algorithm terminates in step 2 if a sink has been reached. We only bother to simulate the first nT computation steps of G' and thus the first T computation steps of G with sufficient accuracy. In the following, we describe how this algorithm is implemented.

We construct unidirectional RTMs for steps 2, 4, 6, and 7 with the following additional properties. We ensure that these machines only use the space already allotted on the work tape, that the time can be bounded by $O(1)$ and $O(n)$ for step 2 and 4, resp., and by a polynomial in the length of the advice tape, i. e., $\text{poly}(s, \log(T/\varepsilon))$, for steps 6 and 7. For step 2, we additionally take care that the running time only depends on the length of the node register, but not on the actual contents of the node register. It is not hard to construct these machines from scratch. Furthermore, Lemma 3.5 yields a unidirectional QTM for step 8 that has space and running time bounded by the length of the node register, i. e., $O(\log s)$ and whose running time is independent of the actual contents of the node register.

For constructing the final QTM from these basic RTMs, we apply appropriate versions of the lemmas of Bernstein and Vazirani [11] for dealing with unidirectional nonuniform RTMs and unidirectional nonuniform QTMs. The finite loops are realized as described by Watrous [39]. At the beginning of a loop, we check a starting/stopping condition for the loop and switch the state of being outside or inside the loop, resp., when this condition is met. For the loops beginning in step 3 and 5, we use counters modulo n and k , resp., and check as the starting/stopping condition whether the counter is equal to zero.

Using these tools, we first combine the machines for the steps 4 and 6–11, implementing the loops in step 3 and 5 as described above, to get a QTM M_{3-11} for steps 3–11. The outermost, endless loop is then realized by modifying the RTM for step 2. We use a simple unidirectional RTM constructed from scratch that carries out the described termination check, enters two special states as placeholders depending on the value of cell 1 of the node register, and then restarts its computation. We insert M_{3-11} into the state for the value 0 of cell 1 (non-sink) and replace the state for the value 1 (sink) with the final state q_f of the whole QTM. This yields the desired QTM for simulating G' and thus G .

We note that a space-bounded RTM performing an infinite loop cannot carry out initialization steps before the loop. By our choice of the encoding of the contents of the tracks, we do not need such an initialization. Furthermore, we have ensured that the running time for the body of the outermost loop is the same for all possible classical inscriptions in the node register. Hence, even if the simulated QBP is in a superposition, step 2 is always reached simultaneously for all nodes in the superposition.

Space and time requirements. The space on tracks 1–6 of the work tape is obviously bounded by $O(1)$, $O(\log s)$, $O(\log s)$, $O(\log n)$, $O(\log k) = O(\log s + \log \log(T/\varepsilon))$, and $O(1)$, resp. The space on track 7 is bounded above by the logarithm of the length of the advice string, which is $O(\log s + \log \log(T/\varepsilon))$ as computed above. Since this is also the contribution of the advice string to the space, the overall space complexity is of the same order. We can estimate the running time for simulating one computation step of G' (steps 2–11 of the algorithm) as follows. The running time of steps 4 and 11 is $O(n)$. The running time of steps 6, 7, 9, and 10 is dominated by the length of the advice tape, which is of order $\text{poly}(s, \log(T/\varepsilon))$. Step 8 can be performed in time proportional to the length of the node register, i.e., $O(\log s)$. Hence, also the overall time for one computation step is of order $\text{poly}(s, \log(T/\varepsilon)) = \text{poly}(|G|, \log(T/\varepsilon))$.

Correctness. Let us assume for a moment that the product $U_{i,k-1}(x_i) \cdots U_{i,0}(x_i)$ equals $U_i(x_i)$. Then it is easy to see that steps 4–10 exactly apply $U_i(x_i)$ and that steps 3–11 exactly apply $U_{n-1}(x_{n-1}) \cdots U_0(x_0)$ to the node register. Together with the termination check in step 2 which realizes the projection E'_{cont} to the non-sink nodes of G' , steps 2–11 exactly apply $U_{n-1}(x_{n-1}) \cdots U_0(x_0)E'_{\text{cont}}$ to the node register if the QTM does not stop. Due to the above claim, we know that this simulates n successive computation steps of G' and thus one computation step of the original QBP G .

However, the product $U_{i,k-1}(x_i) \cdots U_{i,0}(x_i)$ is merely an ε' -approximation of $U_i(x_i)$, where $\varepsilon' = \varepsilon/(2nT^2)$. By Proposition 3.6 we may estimate the error in the application of $U_0(x_0), \dots, U_{n-1}(x_{n-1})$ by $n\varepsilon'$. Let $\hat{p}_{G,r}(a, t)$ be the probability that G halts after *exactly* t steps at a sink labeled by $r \in \{0, 1, ?\}$. Let $\hat{p}_{M,r}(a, t)$ be the probability that M halts after *exactly* t iterations of steps 2–11 and outputs r . As remarked above, the error of one iteration of the outer loop is bounded by $n\varepsilon'$. By Lemma 3.7, $|\hat{p}_{G,r}(a, t) - \hat{p}_{M,r}(a, t)| \leq 2t\varepsilon'n \leq \varepsilon/T$ for all $t = 0, \dots, T$. Hence,

$$\left| \sum_{t=0}^T \hat{p}_{G,r}(a, t) - \sum_{t=0}^T \hat{p}_{M,r}(a, t) \right| \leq \sum_{t=0}^T |\hat{p}_{G,r}(a, t) - \hat{p}_{M,r}(a, t)| \leq \varepsilon.$$

Altogether, we have proved that M simulates T steps of G in $\text{poly}(|G|, T, \log(1/\varepsilon))$ steps with accuracy ε . \square

4.2. High-Level Simulation Theorems

Here we use the basic, technical simulations from the last subsection for proving that the logarithm of the size of QBPs and the space complexity of QTMs asymptotically agree for the standard models of QBPs and QTMs. On the way, we investigate the relationship between precision and running time for QBPs. All proofs are given in Section 4.3. We assume throughout this subsection that the logarithm of the size of the considered QBPs and the space complexity of the QTMs are at least logarithmic in the input length.

We begin with a simple corollary from the basic simulations. If we want to apply the approximate simulation of QBPs by QTMs, we have to specify a bound ε on the simulation error and a bound T on the number of simulation steps in advance. These parameters turn up in a term

of $O(\log \log(T/\varepsilon))$ in the space complexity of the simulating machine. If we restrict ourselves to bounded error computation and to exponential running time, Theorem 4.2 immediately yields:

Corollary 4.3: *The logarithm of the size of QBPs and the space complexity of unidirectional nonuniform QTMs are asymptotically equal if both models are restricted to bounded error and exponential running time in the worst case. Furthermore, the classes of functions computable by sequences of QBPs with polynomial size and by unidirectional nonuniform QTMs with logarithmic space are the same if both models are restricted to bounded error and polynomial running time.*

It is obviously practically motivated to work with bounded running time, but it is not clear what kind of bounds can be chosen without restricting the computational power of the space-bounded models considered here. In [38] and implicitly also in [39], Watrous has investigated this question for unidirectional uniform QTMs and has obtained answers analogous to the situation for probabilistic TMs. He has shown that unidirectional uniform QTMs with rational amplitudes and running in space $S(n) = \Omega(\log n)$ have an expected running time that is at most doubly exponential in $S(n)$. This result can be extended to unidirectional uniform QTMs with algebraic amplitudes using the ideas from his later papers [40, 41].

These considerations provide the motivation to look at the relationship between the precision allowed for the amplitudes and the running time also for the nonuniform model of QBPs. It turns out that short amplitudes take over a role analogous to algebraic amplitudes for QTMs.

Theorem 4.4:

- (i) *Sequences of QBPs $(G_n)_{n \in \mathbb{N}}$ with bounded error and short amplitudes and sequences of QBPs $(G'_n)_{n \in \mathbb{N}}$ with bounded error and expected running time $2^{\text{poly}(|G'_n|)}$ have polynomially related size complexities.*
- (ii) *Sequences of QBPs $(G_n)_{n \in \mathbb{N}}$ with unbounded error and short amplitudes can be simulated by sequences of QBPs $(G'_n)_{n \in \mathbb{N}}$ of size $\text{poly}(|G_n|)$ and with expected running time $2^{\text{poly}(|G'_n|)}$.*

Our final and main result of this subsection provides a justification to regard QBPs with short amplitudes as the natural standard variant of the model analogous to QTMs with algebraic amplitudes.

Theorem 4.5: *The logarithm of the size of QBPs with bounded or unbounded error and short amplitudes and the space complexity of unidirectional nonuniform QTMs with algebraic amplitudes and the same type of error are asymptotically equal.*

4.3. Proofs of Theorems 4.4 and 4.5

For the proofs of the theorems we need a couple of technical lemmas, which are concerned with the analysis of a matrix series that describes the acceptance probability of a QBP. Using these lemmas we provide two results on QBPs with short amplitudes, which are the basic tools for proving Theorems 4.4 and 4.5. First, even in the case of unbounded error there is some gap between the error probability and $1/2$. Second, in QBPs with short amplitudes a probabilistic clock can be added by which computations lasting too long are aborted.

For the following, consider an arbitrary QBP G with s nodes. For any fixed input a for G let $U = U(a)$ be a unitary time evolution matrix of G . Recall that E_{cont} is the projection operator in the measurement of the output label which belongs to the result “no label.” Let $D = UE_{\text{cont}}$ and $M = \overline{D} \otimes D$, where \overline{D} denotes the matrix obtained from D by taking the complex conjugate

of each of its entries. Let $N = s^2$ denote the dimension of M and let $|1\rangle, \dots, |N\rangle$ be the standard basis of \mathbb{C}^N . For $v \in \{1, \dots, s\}$, define $i_v = v + s(v-1) \in \{1, \dots, N\}$. Then, for any $v, w \in \{1, \dots, s\}$, $M_{i_w, i_v} = (\langle w| \otimes \langle w|)M(|v\rangle \otimes |v\rangle)$.

Lemma 4.6:

- (i) *The probability that the node w is reached after exactly k computation steps in G when starting at the node v is equal to $(M^k)_{i_w, i_v}$.*
- (ii) *The absolute value of each eigenvalue of M is bounded above by 1.*

Proof. Part (i) follows from $(M^k)_{i_w, i_v} = (\langle w| \otimes \langle w|)(\overline{D}^k \otimes D^k)(|v\rangle \otimes |v\rangle) = (\overline{D}^k)_{w,v} \cdot (D^k)_{w,v} = |((UE_{\text{cont}})^k)_{w,v}|^2$, which is obviously the desired probability.

For part (ii) it suffices to prove that $\|M\| \leq 1$, since $\|M\|$ provides an upper bound on the absolute value of the eigenvalues of M (see, e.g., [15], page 45). We have $M^\dagger M = (\overline{D} \otimes D)^\dagger (\overline{D} \otimes D) = ((\overline{D})^\dagger \overline{D}) \otimes (D^\dagger D)$. Furthermore, $D^\dagger D = (UE_{\text{cont}})^\dagger (UE_{\text{cont}}) = E_{\text{cont}}^\dagger E_{\text{cont}} = E_{\text{cont}}$. The eigenvalues of $D^\dagger D$ are thus from $\{0, 1\}$, and the same holds for $(\overline{D})^\dagger \overline{D}$. Since the eigenvalues of $M^\dagger M$ are obtained as products of the eigenvalues of $(\overline{D})^\dagger \overline{D}$ and $D^\dagger D$, it follows that $\|M\| \leq 1$. \square

The above lemma yields that, for each pair of nodes (v, w) in G , $\lim_{k \rightarrow \infty} (\sum_{\ell=0}^k M^\ell)_{i_w, i_v}$ is the probability of reaching node w from node v in G . In particular, the acceptance probability of G can be expressed as the sum of all such terms where v is the start node and w is a 1-sink.

We use the technique of Watrous [39, 40, 41] to analyze the series $(\sum_{\ell=0}^\infty M^\ell)_{i_w, i_v}$. Since the matrix series $\sum_{\ell=0}^\infty M^\ell$ does not converge in general, we look at the series $\sum_{\ell=0}^\infty (zM)^\ell$ for some $z \in [0, 1)$ instead and let z tend to 1 afterwards. Using the restrictions on the involved numbers, we then show two facts: First, $\lim_{z \uparrow 1} (\sum_{\ell=0}^\infty (zM)^\ell)_{i_w, i_v}$ can be approximated with sufficient precision by choosing $z = 1 - 2^{-\text{poly}(N)}$. Second, if the limit $(\sum_{\ell=0}^\infty M^\ell)_{i_w, i_v}$ is not exactly $1/2$, then it can be bounded away from $1/2$ by a gap of size at least $2^{-\text{poly}(N)}$.

For a multivariate polynomial f , the *height of f* , denoted by $\|f\|$, is the maximum absolute value of any of its coefficients and $\deg(f)$ is the maximum degree of f with respect to any of its variables. Using the form of the entries of $U = U(a)$ obtained by Proposition 2.9, it is easy to see that there is a real algebraic number α not depending on N and a number $m = 2^{\text{poly}(N)}$ such that each entry of $M = \overline{UE_{\text{cont}}} \otimes UE_{\text{cont}}$ can be written as $p(\alpha)/m$ for an integer polynomial p with $\deg(p) = \text{poly}(N)$ and $\|p\| = 2^{\text{poly}(N)}$. The following three technical lemmas yield properties of general matrices of this form (not necessarily derived from QBPs). The first two lemmas are extracted from [41] (Lemma 4.6 and its proof and the beginning of the proof of Lemma 4.2, resp.).

Lemma 4.7 ([41]): *Let α be any real algebraic number.*

- (i) *If f is a univariate polynomial with $\|f\| \leq 2^d$, $\deg(f) \leq d$ and $f(\alpha) \neq 0$, then $|f(\alpha)| \geq 2^{-O(d^2)}$.*
- (ii) *Let f, g be bivariate integer polynomials with $\|f\|, \|g\| \leq 2^d$, $\deg(f), \deg(g) \leq d$ and $g(\alpha, 1) \neq 0$. Then there is a constant $c > 0$ such that for any δ with $0 < \delta < 2^{-cd^2}$ and d sufficiently large,*

$$\left| \frac{f(\alpha, 1)}{g(\alpha, 1)} - \frac{f(\alpha, 1 - \delta)}{g(\alpha, 1 - \delta)} \right| \leq \delta 2^{cd^2}.$$

Lemma 4.8 ([41]): Let α be any real algebraic number and let $m \in \mathbb{R}$. Let M be an $N \times N$ -matrix such that for each entry x there is an integer polynomial p with $x = p(\alpha)/m$ and $\deg(p) = \text{poly}(N)$, $\|p\| = 2^{\text{poly}(N)}$. Further suppose that the eigenvalues of M are bounded above in absolute value by 1. Let $1 \leq i, j \leq N$ and let $S = \left(\sum_{\ell=0}^{\infty} M^{\ell}\right)_{i,j}$ be convergent. For $z \in [0, 1)$, define $\tilde{S}(z) = \left(\sum_{\ell=0}^{\infty} (zM)^{\ell}\right)_{i,j}$. Then there are bivariate integer polynomials f, g such that $\|f\|, \|g\| \leq m^N 2^{\text{poly}(N)}$, $\deg(f), \deg(g) = \text{poly}(N)$, $g(\alpha, 1) \neq 0$, and

$$\begin{aligned} f(\alpha, z)/g(\alpha, z) &= \tilde{S}(z), \text{ for } z \in [0, 1), \text{ and} \\ f(\alpha, 1)/g(\alpha, 1) &= S. \end{aligned}$$

Lemma 4.9: Let $m = 2^{\text{poly}(N)}$. Let M be an $N \times N$ -matrix as in the previous lemma. Let $S_{i,j} = \left(\sum_{\ell=0}^{\infty} M^{\ell}\right)_{i,j}$ for $1 \leq i, j \leq N$.

- (i) Suppose that $S_{i,j}$ converges. For $z \in [0, 1)$, let $\tilde{S}_{i,j}(z) = \left(\sum_{\ell=0}^{\infty} (zM)^{\ell}\right)_{i,j}$. Then there is a polynomial p such that for any $z = 1 - \delta$ with $0 < \delta < 2^{-p(N)}$, $|S_{i,j} - \tilde{S}_{i,j}(z)| \leq \delta 2^{p(N)}$.
- (ii) Let $I \subseteq \{1, \dots, N\}^2$ and suppose that for each $(i, j) \in I$, $S_{i,j}$ converges. Let $S = \sum_{(i,j) \in I} S_{i,j}$. Then there is a polynomial p such that $S \neq 1/2$ implies $|S - 1/2| \geq 2^{-p(N)}$.

Proof. Part (i): Use Lemma 4.8 to get bivariate integer polynomials $f_{i,j}, g_{i,j}$ such that

$$\begin{aligned} f_{i,j}(\alpha, z)/g_{i,j}(\alpha, z) &= \tilde{S}_{i,j}(z), \text{ for } z \in [0, 1), \text{ and} \\ f_{i,j}(\alpha, 1)/g_{i,j}(\alpha, 1) &= S_{i,j}. \end{aligned}$$

By the lemma and the fact $m = 2^{\text{poly}(N)}$, there is a polynomial q such that $\|f_{i,j}\|, \|g_{i,j}\| \leq 2^{q(N)}$ and $\deg(f_{i,j}), \deg(g_{i,j}) \leq q(N)$ and, furthermore, $g_{i,j}(\alpha, 1) \neq 0$. By Lemma 4.7(ii) applied to $f_{i,j}$ and $g_{i,j}$ with $d = q(N)$, it follows that there is a constant $c > 0$ such that for all $0 < \delta < 2^{-cq(N)^2}$ and N sufficiently large,

$$|S_{i,j} - \tilde{S}_{i,j}(1 - \delta)| = \left| \frac{f_{i,j}(\alpha, 1)}{g_{i,j}(\alpha, 1)} - \frac{f_{i,j}(\alpha, 1 - \delta)}{g_{i,j}(\alpha, 1 - \delta)} \right| \leq \delta 2^{cq(N)^2}.$$

Choosing $p(N) = cq(N)^2$ yields the desired bound for any $z = 1 - \delta$ with $0 < \delta < 2^{-p(N)}$.

Part (ii): By Lemma 4.8, it follows that for each $(i, j) \in I$,

$$S_{i,j} = \left(\sum_{\ell=0}^{\infty} M^{\ell}\right)_{i,j} = \frac{f_{i,j}(\alpha, 1)}{g_{i,j}(\alpha, 1)},$$

where $f_{i,j}$ and $g_{i,j}$ are bivariate integer polynomials with $\|f_{i,j}\|, \|g_{i,j}\| \leq 2^{q(N)}$ and $\deg(f_{i,j}), \deg(g_{i,j}) \leq q(N)$ for some polynomial q , and $g_{i,j}(\alpha, 1) \neq 0$ for all $i, j \in I$. Then

$$S = \sum_{(i,j) \in I} \frac{f_{i,j}(\alpha, 1)}{g_{i,j}(\alpha, 1)} \neq 1/2 \Rightarrow 2 \sum_{(i,j) \in I} f_{i,j}(\alpha, 1) \prod_{(i',j') \neq (i,j)} g_{i',j'}(\alpha, 1) - \prod_{(i,j) \in I} g_{i,j}(\alpha, 1) \neq 0.$$

The left hand side of the last inequality is a polynomial in α with height at most $2^{O(|I| \cdot q(N))} = 2^{\text{poly}(N)}$ and degree at most $|I| \cdot q(N) = \text{poly}(N)$, since $|I| \leq N^2$. Lemma 4.7(i) implies that the absolute value of this expression is lower bounded by $2^{-q'(N)}$ for a suitable polynomial q' and N large enough. Hence,

$$\left| \sum_{(i,j) \in I} \frac{f_{i,j}(\alpha, 1)}{g_{i,j}(\alpha, 1)} - \frac{1}{2} \right| \geq \frac{2^{-q'(N)-1}}{\prod_{(i,j) \in I} |g_{i,j}(\alpha, 1)|}.$$

We have $\|g_{i,j}\| \leq 2^{q(N)}$, $\deg(g_{i,j}) \leq q(N)$, and $\alpha, \alpha^2, \dots, \alpha^{q(N)} = 2^{\text{poly}(N)}$ since α is a constant. This implies that $|g_{i,j}(\alpha, 1)| \leq 2^{q''(N)}$ for a polynomial q'' and N sufficiently large. Thus,

$$|S - 1/2| \geq \frac{2^{-q'(N)-1}}{2^{|I| \cdot q''(N)}} \geq 2^{-p(N)}$$

for $p(N) = q'(N) + N^2 q''(N) + 1$, which proves the claim. \square

Now we can state and prove our first main lemma that allows us to bound the error probability of QBPs away from $1/2$.

Lemma 4.10: *For each QBP G with short amplitudes there exists a polynomial q such that for each input $a \in \{0, 1\}^n$, $p_{G,1}(a) > 1/2$ implies $p_{G,1}(a) \geq 1/2 + 2^{-q(|G|)}$ and $p_{G,1}(a) < 1/2$ implies $p_{G,1}(a) \leq 1/2 - 2^{-q(|G|)}$.*

Proof. Let G be a QBP with short amplitudes on n variables. By Proposition 2.9 we may assume that the amplitudes in G are of the form $p(\alpha)/m$, where p is an integer polynomial with $\deg(p) = \text{poly}(|G|)$ and $\|p\| = 2^{\text{poly}(|G|)}$ and where α is the same algebraic number and $m = 2^{\text{poly}(|G|)}$ is the same natural number for all amplitudes. Let v be the start node of G and let $F_1 = \{w \mid w \text{ is a 1-sink of } G\}$. Let $N = |G|^2$ and let the $N \times N$ -matrix M describing the computation of G on an input $a \in \{0, 1\}^n$ as well as the indices $i_v \in \{1, \dots, N\}$ corresponding to nodes $v \in \{1, \dots, |G|\}$ be defined as above. Then the probability of G accepting a in the k th computation step is given by $\sum_{w \in F_1} (M^k)_{i_w, i_v}$, and the total probability of accepting a is $p_{G,1}(a) = \sum_{w \in F_1} (\sum_{k=0}^{\infty} M^k)_{i_w, i_v}$. Since G only contains labels of the form $p(\alpha)/m$, the entries of M are of the form $p'(\alpha)/m'$, where p' is a polynomial with $\deg(p') = \text{poly}(|G|)$ and $\|p'\| = 2^{\text{poly}(|G|)}$ and $m' = m^2 = 2^{\text{poly}(|G|)}$. Hence, part (ii) of Lemma 4.9 yields the claimed result. \square

The other main argument in our proofs is the construction of a probabilistic clock, which works in the case of bounded as well as unbounded error.

Lemma 4.11: *For each sequence of QBPs $(G_n)_{n \in \mathbb{N}}$ with bounded or unbounded error and short amplitudes, there is a sequence of QBPs $(G'_n)_{n \in \mathbb{N}}$ for the same function with short amplitudes, the same type of error, size $\text{poly}(|G_n|)$, and expected running time $2^{\text{poly}(|G'_n|)}$.*

Proof. The main idea is similar to that of Simon [36] for limiting the running time of probabilistic Turing machines. We simulate G step-by-step. Before each simulation step, we stop and reject the input with fixed, small probability. A similar construction for unidirectional QTMs has been given in Lemma 4.6 of Watrous [39].

Let G be a QBP on n variables of size s . By Proposition 2.9 we may assume that the amplitudes of G are the fraction of some integer polynomial in an algebraic number and a common denominator $m = 2^{\text{poly}(s)}$. Let q be some polynomial. We construct a QBP G' with size polynomial in s , expected running time $2^{\text{poly}(s)}$, and such that for all $a \in \{0, 1\}^n$, $p_{G,1}(a) - 2^{-q(s)} \leq p_{G',1}(a) \leq p_{G,1}(a)$. Together with Lemma 4.10, this implies the claim.

Let $t = t(s) = q(s) + p(s) + \log s$, where $p(s)$ is a polynomial defined later on. Let v_1, \dots, v_s be the nodes of G . The new QBP G' is obtained from the QBP G'_0 shown schematically in Figure 3. We use unlabeled nodes introduced in Section 2 to simplify the presentation. The start node of G'_0 is w_1 . The edges in the upper part of the figure represent the transformation $|w_i\rangle \mapsto \beta|w'_i\rangle + \gamma|w_i^*\rangle$, where

$$\beta = \frac{2^{2t+1} + 2^{t+1}}{2^{2t+1} + 2^{t+1} + 1} \quad \text{and} \quad \gamma = \frac{2^{t+1} + 1}{2^{2t+1} + 2^{t+1} + 1}.$$

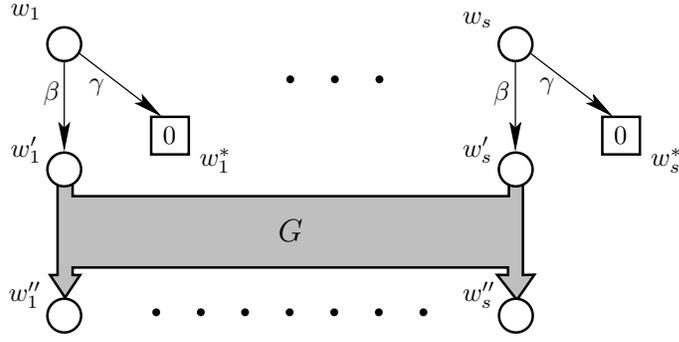


Figure 3: The QBP G'_0 used in the proof of Lemma 4.11.

Then $\beta^2 + \gamma^2 = 1$, which is used to prove that the QBP is well-formed. Each node w'_i , $i \in \{1, \dots, s\}$, is a copy of the node v_i in G and is labeled by the same variable as v_i . For each edge (v_i, v_j) in G , an edge (w'_i, w'_j) is inserted in G'_0 that carries the same labels. The shaded part in the figure represents these edges. The node w'_i is a sink if the corresponding node v_i in G is, and each non-sink node w'_i is unlabeled and has an outgoing edge with amplitude 1 to node w_i (not shown in the figure). The only nodes labeled by variables are w'_1, \dots, w'_s , all other nodes are unlabeled. We remove all unlabeled nodes from G'_0 to obtain the desired QBP G' . It is easy to see that G' constructed in this way is well-formed and unidirectional. The only numbers added as amplitudes here, 1, β , and γ , are rational and have representations of polynomial length. Hence, G' also has short amplitudes.

We observe that the probability of G' terminating during a traversal of the upper part is $\delta = |\gamma|^2 \leq 2^{-2t}$. Hence, its expected running time is bounded by $2^{O(t)} = 2^{\text{poly}(s)}$. Furthermore, for all inputs $a \in \{0, 1\}^n$, $p_{G',1}(a) \leq p_{G,1}(a)$. It remains to show that for all inputs a , $p_{G',1}(a) \geq p_{G,1}(a) - 2^{-q(s)}$.

Fix any input $a \in \{0, 1\}^n$. Let $N = s^2$, let the $N \times N$ -matrix M describing the computation of the original QBP G on a , and let the mapping of nodes $v \in \{1, \dots, s\}$ to indices $i_v \in \{1, \dots, N\}$ be defined as above. Let v be the start node of G and let $F_1 = \{w \mid w \text{ is a 1-sink of } G\}$. As in the proof of Lemma 4.10, the total probability of G accepting a is $p_{G,1}(a) = \sum_{w \in F_1} \left(\sum_{k=0}^{\infty} M^k \right)_{i_w, i_v}$. Now recall that G' performs the same computation as G with the only exception that it terminates the computation with the probability δ before each step of G . Hence, the probability of G' accepting a in the k th simulation step of G after not rejecting k times in the first phase of the computation is $\sum_{w \in F_1} \left((1 - \delta)^k M^k \right)_{i_w, i_v}$. We obtain

$$p_{G',1}(a) = \sum_{w \in F_1} \left(\sum_{k=0}^{\infty} (1 - \delta)^k M^k \right)_{i_w, i_v}.$$

Now choose p as the polynomial obtained when Lemma 4.9(i) is applied with $z = 1 - \delta$, $S_{i,j} = p_{G,1}(a)$, and $\tilde{S}_{i,j}(z) = p_{G',1}(a)$. The lemma implies that

$$|p_{G',1}(a) - p_{G,1}(a)| \leq \sum_{w \in F_1} \left| \left(\sum_{k=0}^{\infty} (1 - \delta)^k M^k \right)_{i_w, i_v} - \left(\sum_{k=0}^{\infty} M^k \right)_{i_w, i_v} \right| \leq |F_1| \cdot \delta \cdot 2^{p(s)},$$

provided that $0 < \delta < 2^{-p(s)}$. The restriction on δ is easily seen to be satisfied since $\delta \leq 2^{-2t}$ and $t = t(s) = p(s) + q(s) + \log s$. Using that $|F_1| \leq s$, we obtain

$$|F_1| \cdot \delta \cdot 2^{p(s)} \leq |F_1| \cdot 2^{-2(q(s)+p(s)+\log s)} \cdot 2^{p(s)} \leq 2^{-q(s)}$$

and thus $|p_{G',1}(a) - p_{G,1}(a)| \leq 2^{-q(s)}$. Hence, G' has all required properties. \square

Now we have collected all tools for the proofs of Theorems 4.4 and 4.5. For the convenience of the reader, we restate the theorems here. We begin with the proof of Theorem 4.5.

Theorem 4.5 (restatement): *The logarithm of the size of QBPs with bounded or unbounded error and short amplitudes and the space complexity of unidirectional nonuniform QTMs with algebraic amplitudes and the same type of error are asymptotically equal.*

Proof. A simulation of unidirectional nonuniform QTMs by QBPs is already provided in Theorem 4.2. It is easy to see that the resulting QBP has short amplitudes if the amplitudes of the QTM are algebraic numbers.

Now let a sequence $(G_n)_{n \in \mathbb{N}}$ of QBPs with short amplitudes be given. By Lemma 4.11 we can simulate G_n by a QBP G'_n with size $\text{poly}(|G_n|)$, the same type of error, short amplitudes and expected running time $T(n) = 2^{\text{poly}(|G'_n|)}$. In the case of bounded error, let ε be the error bound of G'_n . In the case of unbounded error, by Lemma 4.10, there is some polynomial $q(n)$ such that the acceptance and rejection probabilities of G'_n are strictly larger than $1/2 + 2^{-q(|G'_n|)}$ or strictly smaller than $1/2 - 2^{-q(|G'_n|)}$, resp. In this case let $\varepsilon = \varepsilon(n) = 1/2 - 2^{-q(|G'_n|)}$ be the error bound of G'_n . We choose $\varepsilon' = (1/2 - \varepsilon)/3$ and $T'(n) = T(n)/\varepsilon' = 2^{\text{poly}(|G'_n|)}$. Then we apply the simulation of QBPs by QTMs from Theorem 4.2 for the accuracy ε' and the running time $T'(n)$. The space complexity of the QTM is $O(\log |G'_n| + \log \log(T'(n)/\varepsilon')) = O(\log |G_n|)$. By Markov's inequality, the probability that the running time of G'_n and thus the number of performed simulation steps exceeds $T'(n) = T(n)/\varepsilon'$ is bounded by ε' . Hence, the probability of an error caused by running more than $T'(n)$ simulation steps is bounded by ε' and the overall error probability is bounded by $\varepsilon + 2\varepsilon' = 1/2 - \varepsilon'$. \square

Theorem 4.4 (restatement):

- (i) *Sequences of QBPs $(G_n)_{n \in \mathbb{N}}$ with bounded error and short amplitudes and sequences of QBPs $(G'_n)_{n \in \mathbb{N}}$ with bounded error and expected running time $2^{\text{poly}(|G'_n|)}$ have polynomially related size complexities.*
- (ii) *Sequences of QBPs $(G_n)_{n \in \mathbb{N}}$ with unbounded error and short amplitudes can be simulated by sequences of QBPs $(G'_n)_{n \in \mathbb{N}}$ of size $\text{poly}(|G_n|)$ and with expected running time $2^{\text{poly}(|G'_n|)}$.*

Proof. A simulation of QBPs $(G_n)_{n \in \mathbb{N}}$ with short amplitudes by QBPs $(G'_n)_{n \in \mathbb{N}}$ with expected running time $2^{\text{poly}(|G'_n|)}$ for bounded and unbounded error is contained in Lemma 4.11. This proves one direction of part (i) as well as part (ii). It remains to prove the missing direction of part (i), i. e., to provide a simulation of QBPs with bounded error and an expected exponential running time by QBPs with bounded error and short amplitudes. Let $(G_n)_{n \in \mathbb{N}}$ be a sequence of QBPs with expected running time $2^{\text{poly}(|G_n|)}$ and error probability $\varepsilon \in [0, 1/2)$. As in the proof of Theorem 4.5, we choose $\varepsilon' = (1/2 - \varepsilon)/3$ and $T'(n) = T(n)/\varepsilon' = 2^{\text{poly}(|G_n|)}$ and apply the simulation of QBPs by QTMs of Theorem 4.2 for the accuracy ε' and the running time $T'(n)$. By the same arguments as in the proof of Theorem 4.5, we obtain a unidirectional nonuniform QTM simulating the given QBP with bounded error, expected running time $T(n)$, and space complexity $O(\log |G_n|)$. The transition function of the QTM only contains a constant number of algebraic numbers.

In a second step we apply the simulation of unidirectional nonuniform QTMs by QBPs from Theorem 4.2. The resulting QBP has an error probability of at most ε' . Its size is bounded above by $2^{O(\log |G_n|)} = \text{poly}(|G_n|)$. The amplitudes occurring in the QBP are the amplitudes of the transition function of the QTM and thus are short. \square

5. Simulation of Nonuniform QTMs by Unidirectional Nonuniform QTMs

In this section, we consider nonuniform RTMs and QTMs that are, different from the previous sections, not necessarily unidirectional. We show that they can be simulated space-efficiently by their unidirectional counterparts. We discuss some consequences of the simulation result at the end of this section.

Our simulation result uses the construction of the universal QTM due to Yao [43] and Nishimura and Ozawa [27] based on a simulation of QTMs by quantum circuits and vice versa as intermediate steps. The original simulations cannot be applied since they use markers on the work tape of the simulating machine to store the positions of the simulated tape heads and (which is more serious) generate a quantum circuit for the simulated machine online on the work tape. Both of this is too costly in terms of space. These obstacles are overcome here by using a space-efficient encoding of the positions of the input tape heads and by storing a representation of the required quantum circuit on the advice tape.

As a preparation for the proof of our simulation result, we state a simple necessary property of the transition function of QTMs with two read-only input tapes which is extracted from the proof of Theorem 4.5 in [28]. In the following the expression $[A = B]$ has the value 1, if $A = B$, and 0 otherwise.

Lemma 5.1 ([28]): *Let $M = (Q, \Sigma, \delta)$ be a QTM with two read-only input tapes. Let $p, p' \in Q$, $\Delta = (\Delta_1, \Delta_2) \in \mathbb{Z}^2$ and $a_1, a_2, a'_1, a'_2, v, w, v', w' \in \Sigma$.*

$$(i) \quad 0 = \sum_{\substack{q \in Q, d'' \in \{0,1\}, \\ d, d' \in \{-1,0,1\}^2}} \delta(p, (a_1, a_2, v), q, w, (d, d'' - 1))^* \cdot \delta(p', (a'_1, a'_2, v'), q, w', (d', d'')) \cdot [d' - d = \Delta].$$

$$(ii) \quad 0 = \sum_{\substack{q \in Q, \\ d, d' \in \{-1,0,1\}^2}} \delta(p, (a_1, a_2, v), q, w, (d, -1))^* \cdot \delta(p', (a'_1, a'_2, v'), q, w', (d', 1)) \cdot [d' - d = \Delta].$$

Now we can state and prove our result.

Theorem 5.2:

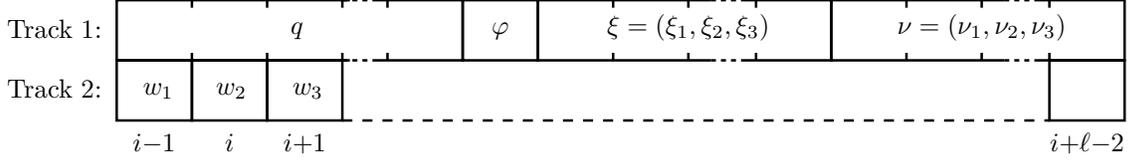
- (i) *Each nonuniform RTM that runs in space S at least logarithmic in the input length and time T can be simulated by a unidirectional nonuniform RTM running in time $\text{poly}(S, T)$ and space $O(S)$.*
- (ii) *Let $\varepsilon > 0$ and $T: \mathbb{N} \rightarrow \mathbb{N}_0$. For each nonuniform QTM M running in space S at least logarithmic in the input length, there is a unidirectional nonuniform QTM that simulates M for T steps in $\text{poly}(2^{O(S)}, T, \log(1/\varepsilon))$ steps with accuracy ε using space $O(S + \log \log(T/\varepsilon))$.*

Proof. In the main part of the proof, we deal with part (ii). We handle necessary changes for part (i) and RTMs at the end. We first describe how we encode the information about the simulated machine on the work tape of the simulating machine. Then we present a high-level algorithm carrying out a whole simulation step and define a unitary transformation realizing a single transition of the simulated machine. Afterwards, this unitary transformation is implemented approximately by the simulating unidirectional nonuniform QTM.

Storage layout on the work tape. Let $M = (Q, \Sigma, \delta)$ be a nonuniform QTM that is to be simulated unidirectionally. We regard the advice tape simply as an additional read-only input tape. We assume that for input length n and space bound $S \geq \log n$ the heads on the input

tapes $i \in \{1, 2\}$ of M only reach the positions $0, \dots, n_i - 1$, where $n_1 = n + 2$, $n_2 = \text{poly}(n)$, and that the work tape head only reaches the positions $0, \dots, n_3 - 1$ with $n_3 = S + 2$ (this may be achieved using end markers). We assume that $\{0, 1, 2\} \subseteq \Sigma$.

Let $\ell = \ell_1 + 6\ell_2 + 1$ with $\ell_1 = \lceil \log |Q| \rceil$ and $\ell_2 = \max\{\lceil \log n_i \rceil \mid i \in \{1, 2, 3\}\} = O(S)$, and assume w. l. o. g. that $\ell \geq 3$. The information about the simulated machine is stored on two tracks of the work tape of the simulating machine as shown below.



Track 2 contains the work tape of the simulated machine. In ℓ consecutive cells on track 1, which are called the *info block*, we encode all administrative information for the simulation. The position of the info block is used to indicate the position of the head on the work tape in a classical configuration. If the cells of the info block are located at positions $i - 1, i, i + 1, \dots, i + \ell - 2$ on the work tape as shown in the figure, we say that the info block is at position i . In this situation, the inscription in the info block together with the symbols $w_1, w_2, w_3 \in \Sigma$ in cells $i - 1, i, i + 1$ on track 2 are called the *info window* induced by the info block.

The information stored in the info block consists of the local state $q \in Q$ of the simulated machine encoded in binary, a flag $\varphi \in \{0, 1\}$ showing whether the actual transition step has already been carried out, and vectors $\xi = (\xi_1, \xi_2, \xi_3), \nu = (\nu_1, \nu_2, \nu_3)$ in $\{0, \dots, n_1 - 1\} \times \dots \times \{0, \dots, n_3 - 1\}$ encoded in binary. The coordinates of ξ are the positions of the tape heads of the simulated machine. Similarly, ν_1 and ν_2 are the positions of the heads on the input tapes of the simulating machine. Finally, ν_3 is the position of the info block. We write the contents of the info window shown above as $(q, \varphi, \xi, \nu, w)$, where $w = (w_1, w_2, w_3)$.

Carrying out a simulation step. We first give an outline of our approach. For the simulation of a single step of M , we let the input tape heads of the simulating machine as well as the info block on the work tape successively move to all combinations of positions in $\{0, \dots, n_1 - 1\} \times \dots \times \{0, \dots, n_3 - 1\}$ on the tapes that may be accessed. If during this sweep the machine reaches a configuration where the positions of the heads of the input tapes as well as the position of the info block, which are encoded in ν , all agree with the stored positions of those of the simulated machine and $\varphi = 0$, then a local transition of the simulated machine is applied, for which we update the contents of the info window and set $\varphi = 1$. After the sweep through all positions is complete, the flag φ is negated.

In Figure 4 this is described in more detail as a high-level algorithm. We use the following notation. For $x = (x_1, x_2, x_3) \in \{0, \dots, n_1 - 1\} \times \dots \times \{0, \dots, n_3 - 1\}$, let $|x| = x_3 n_2 n_1 + x_2 n_1 + x_1$. Furthermore, let $|q, \varphi, \xi, \nu, w_1 w_2 w_3\rangle$ denote an ON-basis indexed by the different possible classical inscriptions of the info window.

Realizing a Transition Unitarily. Next we show that step 2 of the high-level algorithm can be described by a unitary transformation. For this, let the heads on the input tapes of the simulating machine as well as the info block on the work tape be at fixed positions. Let $a_1, a_2 \in \Sigma$ be the symbols under the input tape heads. Our goal is to specify a unitary transformation $U_{\text{trans}} = U_{\text{trans}}(a_1, a_2)$ that changes the contents of the info window according to the high-level algorithm. Using an idea due to Yao [43], we only carry out the identity in step 2.2 for those inscriptions of the info window that can actually arise during the computation at this point.

Loop with starting/stopping condition $\nu = (0, 0, 0)$:

1. Move the real input tape heads and the info block on the work tape to the positions in ν .
2. Transition: Let $(p, \varphi, \xi, \nu, (w_1, w_2, w_3))$ be the contents of the current info window and let $a_1, a_2 \in \Sigma$ be the symbols under the input tape heads.

2.1. If $\xi = \nu$ and $\varphi = 0$, replace the contents of the info window with the superposition

$$\sum_{\substack{q \in Q, b \in \Sigma, \\ d \in \{-1, 0, 1\}^3}} \delta(p, (a_1, a_2, w_2), q, b, d) |q, 1, \xi + d, \xi, w_1 b w_3\rangle.$$

2.2. For all inscriptions of the info window that do not satisfy the condition of step 2.1 and can actually arise during the computation, do nothing.

3. Move real input tape heads and the info block on the work tape to positions $(0, 0, 0)$.

4. Update ν to a new vector ν' such that $|\nu'| \equiv (|\nu| + 1) \bmod n_1 \cdot n_2 \cdot n_3$.

Set $\varphi = 1 - \varphi$. End of simulation step.

Figure 4: High-level description of the simulation step.

$$\begin{aligned} |v_{p, \xi, w_1, w_2, w_3}^{(1)}\rangle &= |p, 0, \xi, \xi, w_1 w_2 w_3\rangle \\ |v_{p, \xi, w_1, w_2, w_3}^{(2)}\rangle &= \sum_{q, b, d} \delta(p, (a_1, a_2, w_2), q, b, d) |q, 1, \xi + d, \xi, w_1 b w_3\rangle \\ |v_{p, \xi, \nu, w_1, w_2, w_3}^{(3)}\rangle &= |p, \varphi, \xi, \nu, w_1 w_2 w_3\rangle \text{ with } \varphi = 0 \wedge \nu \neq \xi \text{ or } \varphi = 1 \wedge \nu_3 \geq \xi_3 + 2 \\ |v_{p, \xi, \nu_1, \nu_2, w, w_2, w_3}^{(4)}\rangle &= \sum_{\substack{q, b, d \text{ with} \\ d_3 \in \{0, 1\}}} \delta(p, (a_1, a_2, w), q, b, d) |q, 1, \xi + d, (\nu_1, \nu_2, \xi_3 + 1), b w_2 w_3\rangle \\ |v_{p, \xi, \nu_1, \nu_2, w, b, w_1, w_2, w_3}^{(5)}\rangle &= \sum_{\substack{q, d \text{ with} \\ d_3 = 1}} \delta(p, (a_1, a_2, w), q, b, d) |q, 1, \xi + d, (\nu_1, \nu_2, \xi_3 + 2), w_1 w_2 w_3\rangle \end{aligned}$$

Figure 5: Vectors for the definition of U_{trans} .

This is required to allow the transformations of steps 2.1 and 2.2 to be combined to a unitary one.

For a precise definition of U_{trans} , we introduce the collections of vectors in Figure 5. For these definitions, let $p \in Q$, $\xi = (\xi_1, \xi_2, \xi_3)$, $\nu = (\nu_1, \nu_2, \nu_3) \in \{0, \dots, n_1 - 1\} \times \dots \times \{0, \dots, n_3 - 1\}$, and $w, b, w_1, w_2, w_3 \in \Sigma$. The summations are over all $q \in Q$, $b \in \Sigma$, and $d = (d_1, d_2, d_3) \in \{-1, 0, 1\}^3$ if not indicated otherwise. Let V_i be the set of vectors with upper index $i \in \{1, \dots, 5\}$.

We require that the transformation U_{trans} satisfies

$$U_{\text{trans}} |v_{p, \xi, w_1, w_2, w_3}^{(1)}\rangle = |v_{p, \xi, w_1, w_2, w_3}^{(2)}\rangle$$

for all p, ξ , and w_1, w_2, w_3 and that $U_{\text{trans}} |v\rangle = |v\rangle$ for all $|v\rangle \in V_3 \cup V_4 \cup V_5$. The following claim implies that the above requirements can be satisfied by a unitary operator U_{trans} , completing this part of the proof.

Claim. The sets V_1 , V_2 , and $V_3 \cup V_4 \cup V_5$ are mutually orthogonal and the vectors in V_2 form an ON-basis.

Proof of the claim. The claim follows from the fact that M is a legal QTM and thus has a unitary time evolution operator. We use the notion “superposition of M ” to describe a unit vector from the Hilbert space spanned by the classical configurations of M as an ON-basis.

The vectors in V_2 form an ON-basis: We regard the vectors in V_1 and V_2 as unique descriptions of superpositions of M . This is possible since the contents of the work tape of M that is outside the three symbols in the info window is fixed. Each vector $|v_{p,\xi,w_1,w_2,w_3}^{(2)}\rangle$ uniquely describes the image of the classical configuration described by $|v_{p,\xi,w_1,w_2,w_3}^{(1)}\rangle$ under the time evolution operator of M . Since this time evolution operator is unitary and the vectors in V_1 obviously form an ON-basis, the vectors from V_2 also form an ON-basis.

The vectors in V_1 , V_2 , $V_3 \cup V_4 \cup V_5$ are mutually orthogonal: We write $M_1 \perp M_2$ for two sets of vectors M_1 and M_2 if $\langle v | w \rangle = 0$ for all $v \in M_1$ and $w \in M_2$ and prove the statement by considering all possible pairs of sets in the list.

$V_1 \perp V_2$, $V_1 \perp V_3 \cup V_4 \cup V_5$, $V_2 \perp V_3$: This follows immediately, since either the component for the flag φ or that for the position vector ν distinguishes vectors from the considered sets.

$V_2 \perp V_4$: We consider any pair of vectors $|v_{p,\xi,w_1,w_2,w_3}^{(2)}\rangle$ and $|v_{p',\xi',\nu'_1,\nu'_2,w'_1,w'_2,w'_3}^{(4)}\rangle$. We may assume that $w'_3 = w_3$, $\nu'_i = \xi_i$ for $i \in \{1, 2\}$ and $\xi'_3 = \xi_3 - 1$ since otherwise the inner product of these vectors is obviously zero. By keeping only the summands in the inner product for which the basis vectors meet, we get

$$\begin{aligned} \langle v_{p,\xi,w_1,w_2,w_3}^{(2)} | v_{p',(\xi'_1,\xi'_2,\xi_3-1),\xi_1,\xi_2,w',w'_2,w_3}^{(4)} \rangle = \\ \sum_{\substack{q \in Q, d, d' \in \{-1, 0, 1\}^3, \\ \text{with } d'_3 \in \{0, 1\}}} \delta(p, (a_1, a_2, w_2), q, w'_2, d)^* \\ \cdot \delta(p', (a'_1, a'_2, w'), q, w_1, d') \cdot [d' - d = \xi - \xi']. \end{aligned}$$

For the d, d' over which the summation is done, it is required that $d'_3 - d_3 = \xi_3 - \xi'_3 = 1$, i. e., $d_3 = d'_3 - 1$. The sum may thus be rewritten as

$$\sum_{\substack{q \in Q, d'' \in \{0, 1\}, \\ d, d' \in \{-1, 0, 1\}^2}} \delta(p, (a_1, a_2, w_2), q, w'_2, (d, d'' - 1))^* \\ \cdot \delta(p', (a'_1, a'_2, w'), q, w_1, (d', d'')) \cdot [d' - d = (\xi_1, \xi_2) - (\xi'_1, \xi'_2)].$$

For $\Delta = (\xi_1, \xi_2) - (\xi'_1, \xi'_2)$, Lemma 5.1(i) implies that the sum takes the value 0. Thus the considered vectors are orthogonal.

$V_2 \perp V_5$: This case is handled similarly to the latter one now using part (ii) of Lemma 5.1. \square

Constructing the Simulating QTM. We now describe how the QTM simulating the given QTM M unidirectionally is constructed. This simulating QTM carries out an endless loop executing single simulation steps until the simulated machine terminates, similar to the machine constructed for part (ii) of Theorem 4.2. It is initialized as follows.

- The info block belonging to the initial configuration of M is located at position 0 of track 1 of the work tape. The complete contents of the respective info window is then $(q_0, 0, \xi, \nu, w)$, where q_0 is the initial state of M , $\xi = \nu = (0, 0, 0)$, and w only consists of blanks.
- All input tape heads of the simulating machine are at position 0.

As in the last section, this initialization is realized by choosing the encoding for the information on the work tape such that the blank tape is consistent with the above requirements.

We realize the high-level algorithm by first constructing a unidirectional RTM for everything except for step 2, for which the RTM has a special state as a placeholder. This is easy by putting together machines for basic tasks using appropriate versions of the lemmas of Bernstein and Vazirani [11], as in the last section. Afterwards, we insert a QTM for carrying out step 2 which has still to be constructed. We ensure that the running time of this QTM is independent of the inscriptions of the info window. Then the complete QTM for the high-level algorithm obtained by the insertion has a running time independent of the contents of the different tapes.

The transformation U_{trans} operates on a Hilbert space of dimension $O(\ell) = O(S)$. The number of iterations of the loop is $n_1 n_2 n_3 = \text{poly}(n)S$. Reusing the calculations in the proof of Theorem 4.2(ii), it follows that a description of U_{trans} with accuracy $\varepsilon' = \varepsilon/(2n_1 n_2 n_3 T^2)$ by elementary matrices adds $O(S + \log \log(T/\varepsilon))$ to the total space complexity if it is stored on the advice-tape. This is within the required bound for part (ii) of the theorem. The chosen accuracy ε' is sufficient to carry out the T simulation steps with accuracy ε . This corresponds to $n_1 n_2 n_3 T$ executions of U_{trans} . The transformation U_{trans} is realized by carrying out the respective elementary transformations as described in the last section, using Lemma 3.5.

Resources. The running time for carrying out U_{trans} is dominated by the length of its description on the advice tape and can be estimated by $2^{O(S)} \log(T/\varepsilon)$. The number of iterations of the loop is $\text{poly}(n)S$. Thus the total time required for one simulation step can be estimated by $O(\text{poly}(n)2^{O(S)} \log(T/\varepsilon)) = \text{poly}(2^{O(S)}, \log(T/\varepsilon))$.

Correctness. We show that each single computation step is performed correctly. We first consider step 2.1 of the high-level algorithm and the case that the condition in this step is met. We assume that the current configuration of the simulating machine is consistent with our described invariants, that track 2 and the info block contain classical inscriptions, and that the latter is at a fixed position. Then it is easy to see that U_{trans} correctly realizes a single transition of M .

It remains to check that step 2.2 does not change anything. We observe that before the transition of M has been carried out in step 2.1, U_{trans} performs the identity in step 2.2, since all encountered info window inscriptions correspond to vectors from V_3 . Immediately after the transition, the info window operated upon contains a vector $|v\rangle \in V_2$. If after one or two shifts of the info window to the right on the work tape we adapt $|v\rangle$ by inserting the new ν , this yields a vector from V_4 or V_5 , resp., on which U_{trans} also performs the identity. If the window is shifted further to the right, the distance of the info window from the stored position of the work tape head in each classical inscription contained in the current superposition is at least two. Then the vector obtained by adapting $|v\rangle$ as described belongs to V_3 and U_{trans} also performs the identity. Hence, U_{trans} behaves as desired. Altogether, we have completed the proof of part (ii).

Simulation of RTMs. We can use the same construction as above, but replace the implementation of U_{trans} . In this case, U_{trans} is just a permutation of inscriptions of the info window. This permutation can be computed exactly by a reversible circuit of size $\text{poly}(\ell)$ consisting only of Toffoli gates. The description of this circuit on the advice tape adds an amount of $O(\log \ell) = O(\log S)$ to the space complexity and its simulation takes time $\text{poly}(\ell) = \text{poly}(S)$, which yields an overall bound on the time of $\text{poly}(S, T)$. Hence, also part (i) follows. \square

Since the simulation of QTMs in Theorem 5.2 is done only approximately and the space $O(S + \log \log(T/\varepsilon))$ needed for the simulation increases with the running time we again obtain

the question in which cases we can bound the running time without restricting the computational power of the model. Here we need a statement for bounding the error probability away from $1/2$ in the case of unbounded error and a construction of a probabilistic clock for QTM.

Lemma 5.3: *For each nonuniform QTM M with algebraic amplitudes and running in space $S(n)$ there exists a polynomial q such that for each input $a \in \{0,1\}^n$, $p_{M,1}(a) > 1/2$ implies $p_{M,1}(a) \geq 1/2 + 2^{-q(2^{S(n)})}$ and $p_{M,1}(a) < 1/2$ implies $p_{M,1}(a) \leq 1/2 - 2^{-q(2^{S(n)})}$.*

Lemma 5.4: *For each nonuniform QTM M with bounded or unbounded error, algebraic amplitudes and running in space $S(n)$, there is a QTM for the same function with algebraic amplitudes, the same type of error, the space bound $O(S(n))$ and expected running time $2^{2^{O(S(n))}}$.*

Lemma 5.3 is proved in the same way as Lemma 4.10 since the matrix describing the transition probabilities in the proof in the same way describes transition probabilities of nonuniform QTM. For the proof of Lemma 5.4 we modify the given QTM M in a way similar to the construction of the QBP in the proof of Lemma 4.11. Using the proof of Lemma 4.6 in Watrous [39] it is easy to construct a QTM M_t that for an appropriate $t = 2^{O(S)}$ stops with probability $2^{-\Theta(t)}$ and continues with probability $1 - 2^{-\Theta(t)}$. Using suitable versions of the lemmas of Bernstein and Vazirani [11] for the construction of QTM we modify M in such a way that, before each computation step, it additionally performs M_t . By a reasoning similar to the proof of Lemma 4.11 we obtain a QTM with the behavior claimed in Lemma 5.4. Using these results we easily obtain the following.

Theorem 5.5: *The space complexity of nonuniform QTM with algebraic amplitudes and bounded or unbounded error is asymptotically equal to the space complexity of unidirectional nonuniform QTM with the same kind of amplitudes and the same type of error, provided that these space complexities are at least logarithmic in the input length.*

Proof. Applying Lemmas 5.3 and 5.4 to a nonuniform QTM that according to the hypothesis runs in space S , we obtain a nonuniform QTM of the same kind running in expected time $2^{2^{O(S)}}$. Analogously to the proofs in the last section, using Markov's inequality to estimate the error of computations that take longer than time $2^{2^{O(S)}}$, Theorem 5.2 yields a unidirectional nonuniform QTM of the desired kind running in space $O(S)$. \square

6. Quantum OBDDs

Since for unrestricted branching programs no powerful lower bound methods are known, restricted variants of branching programs have been investigated in order to develop lower bound methods and to compare different modes of nondeterminism and randomization. A simple variant of branching programs closely related to the uniform model of DFAs and to one-way communication complexity are ordered binary decision diagrams (OBDDs). OBDDs are also used as a data structure for the representation and manipulation of boolean functions, see, e. g., Wegener [42]. Hence, it is natural to investigate also the quantum variant of OBDDs.

Definition 6.1: A *quantum OBDD (QOBDD)* is a read-once QBP where on each path the variables are tested according to the same order.

Below, we prove upper and lower bound results for QOBDDs. Before we do that, we discuss the definition of QOBDDs and their relationship to quantum finite automata. Furthermore, we define complexity classes in terms of the size of QOBDDs and compare them with the corresponding complexity classes for OBDDs.

Since on each path from the start node to a sink each variable is tested at most once, QOBDDs are always acyclic. Because of the definition of QBPs, also QOBDDs are unidirectional. Different from Definition 6.1, Ablayev, Gainutdinova, and Karpinski [1] require QOBDDs to be leveled such that there are edges only between adjacent levels. Proposition 2.10 shows that this restriction is not crucial, because QOBDDs according to Definition 6.1 can be transformed into leveled QOBDDs where the size increases by a factor of at most $(n + 1)^2$.

Despite their superficial similarity, there are some important differences between QOBDDs and (1-way) quantum finite automata (QFAs). At the definition level, observe that, unlike QFAs, QOBDDs may read their input in an order different from x_1, \dots, x_n . Furthermore, they are a nonuniform model while QFAs are uniform. This implies two less obvious differences between QOBDDs and QFAs. In general, measuring whether the computation has stopped and, if yes, with which result, is allowed also during the computation of a QOBDD. The more restrictive definition that allows end nodes to be reached only after exactly n computation steps have been performed is equivalent to our definition because of Proposition 2.10. On the other hand, it is known that QFAs with and without such intermediate measurements are of different power (Kondacs and Watrous [20]). Furthermore, one can decrease the error probability of a QOBDD with bounded error by *probability amplification* below any given constant, as for randomized OBDDs (see [42] for the randomized case). Again, this does not work for QFAs: Ambainis and Freivalds [7] have shown that the language $\{a\}^* \{b\}^*$ can be recognized by QFAs with two-sided error 0.318, but not with error smaller than $2/9$.

For QOBDDs, we distinguish the same types of error as for general QBPs (see Definition 2.5). For characterizing the relative power of the resulting different types of QOBDDs, it is useful to define complexity classes with a naming convention analogous to that used for QTMs. The class of functions that can be computed exactly by polynomial size QOBDDs is called EQP-OBDD, and the class of functions with polynomial size zero error (bounded-error) QOBDDs is called ZQP-OBDD (BQP-OBDD). Similarly, the classes P-OBDD and BPP-OBDD of functions with polynomial size deterministic OBDDs and polynomial size randomized OBDDs with bounded error are defined. Furthermore, let Rev-OBDD denote the class of functions with polynomial size reversible OBDDs. The inclusions $\text{Rev-OBDD} \subseteq \text{EQP-OBDD} \subseteq \text{ZQP-OBDD} \subseteq \text{BQP-OBDD}$ and $\text{Rev-OBDD} \subseteq \text{P-OBDD} \subseteq \text{BPP-OBDD}$ immediately follow from the definitions.

In this section we present simple, concrete example functions in order to prove that QOBDDs with bounded error and classical, deterministic OBDDs are incomparable in power, i.e., $\text{P-OBDD} \not\subseteq \text{BQP-OBDD}$ and $\text{BQP-OBDD} \not\subseteq \text{P-OBDD}$. We also present a partially defined function in order to show a similar result for QOBDDs and classical, randomized OBDDs for partial functions. Finally, we study the power of zero error and exact quantum computation for OBDDs. We prove that $\text{ZQP-OBDD} \subseteq \text{Rev-OBDD}$, i.e., zero error QOBDDs can *at best* be as good as reversible OBDDs. This implies that the three classes Rev-OBDD, EQP-OBDD, and ZQP-OBDD coincide and are strictly contained in P-OBDD.

6.1. A Function with Small QOBDDs that Requires Large Deterministic OBDDs

The *permutation matrix test function* PERM_n is defined on n^2 boolean variables that are arranged in a quadratic matrix. The function takes the value 1 iff each row and each column contains exactly one entry 1. It is well-known that $\text{PERM} = (\text{PERM}_n)_{n \in \mathbb{N}}$ does not have polynomial size read-once branching programs (Krause, Meinel and Waack [21]) and, therefore, no polynomial size OBDDs either. In [33] (see also [42]), a polynomial size randomized OBDD with one-sided error for PERM has been designed using the so-called fingerprinting technique. We show here how this construction can be modified to work for QOBDDs.

Let X denote the input matrix and let $x_j = (x_{j,0}, \dots, x_{j,n-1})$ denote the j th row of X . Let $|x_j| = \sum_k x_{j,k} 2^k$ denote the value of the j th row interpreted as a binary number. The crucial observation is that

$$\text{PERM}_n(X) = 1 \Leftrightarrow \sum_{j=0}^{n-1} |x_j| - (2^n - 1) = 0 \wedge \text{each } x_j \text{ contains exactly one entry } 1.$$

The exact evaluation of the sum $S = \sum_{j=0}^{n-1} |x_j| - (2^n - 1)$ requires OBDDs of exponential size. Hence, S is evaluated modulo a randomly chosen prime number p . It is straightforward to construct a reversible OBDD $G^{(p)}$ that evaluates $S \bmod p$ and simultaneously checks that each x_j contains exactly one entry 1. In $G^{(p)}$ the variables are tested in a rowwise order. For each row it has to be stored whether an entry 1 has already been found. If a second 1 is found in some row, a 0-sink is reached. Furthermore, in each level the OBDD stores the partial sum of the terms corresponding to the bits already read. Since the partial sums are only stored modulo p , this increases the width merely by a factor of p . Altogether, each level contains at most $2p$ interior nodes. Hence, the size of $G^{(p)}$ is $O(pn^2)$. It only accepts if $S \bmod p$ is equal to 0.

Now we construct a QOBDD G for PERM_n . Let $m = 2n^2$ and let p_1, \dots, p_m denote the m smallest primes. By the prime number theorem, $p_m = O(m \log m) = O(n^2 \log n)$. We construct $G^{(1)}, \dots, G^{(p_m)}$ and combine these reversible OBDDs by a node labeled by the first variable with m outgoing c -edges with amplitudes $1/\sqrt{m}$ leading to the c -successors of the start nodes of $G^{(1)}, \dots, G^{(p_m)}$. This realizes a random choice between $G^{(p_1)}, \dots, G^{(p_m)}$. The size of G is bounded by $O(n^6 \log n)$.

We estimate the error probability. The sum S is bounded above by $n2^n$. Hence, if S is different from 0, it has at most $n + \log n$ prime factors. Thus the probability of randomly choosing a prime dividing S is bounded above by $(n + \log n)/(2n^2) \leq 1/n$. This is also an upper bound on the error probability of G . The error is one-sided, i. e., if $\text{PERM}_n(X) = 1$, then the QOBDD G always computes 1, while it may err if $\text{PERM}_n(X) = 0$. The probability can even be made smaller than $1/p(n)$ for any polynomial p by increasing the number of primes, which only increases the size of G polynomially. We have proved:

Theorem 6.2: *There are QOBDDs for $\neg \text{PERM}_n$ with one-sided error $1/n$ and size $O(n^6 \log n)$.*

Corollary 6.3: *BQP-OBDD $\not\subseteq$ P-OBDD.*

6.2. Functions with Small Deterministic OBDDs that Require Large QOBDDs

The disjointness function and the inner product function are defined by $\text{DISJ}_n(x_1, \dots, x_n) = (\bar{x}_1 \vee \bar{x}_2) \wedge (\bar{x}_3 \vee \bar{x}_4) \wedge \dots \wedge (\bar{x}_{n-1} \vee \bar{x}_n)$ and $\text{IP}(x_1, \dots, x_n) = x_1 x_2 \oplus \dots \oplus x_{n-1} x_n$, where n is an even number. Both functions are extensively investigated in communication complexity, see, e. g., [22]. For the variable order x_1, \dots, x_n they have OBDD size $O(n)$, since it suffices to store at most two bits at each level of the OBDD, namely, the value of the variable read in the last step and the value that the function takes on the variables up to the last variable with an even index. However, both functions are difficult for QOBDDs and, therefore, also for reversible OBDDs, since these OBDD models have difficulties in “forgetting” variables read.

The lower bound proof uses some ideas due to Nayak [25] based on quantum information theory. We briefly introduce the required notions and facts. For a proper introduction to quantum information theory we refer to [26]. Recall that a *mixed state* of a quantum system is a probability distribution of pure quantum states. A mixed state is usually described by

its *density matrix*, which is a positive matrix with unit trace. The density matrix for the probability distribution $(p_i, |\varphi_i\rangle)_i$ is $\sigma = \sum_i p_i |\varphi_i\rangle\langle\varphi_i|$. A state resulting from the application of the unitary transformation U to the state described by the density matrix σ is described by the density matrix $U\sigma U^\dagger$. Now assume that $(|\psi_i\rangle)_i$ is an orthonormal basis of eigenvectors of σ and that λ_i is the eigenvalue belonging to $|\psi_i\rangle$. Then the *von Neumann entropy* of σ is defined as $S(\sigma) = -\sum_i \lambda_i \log \lambda_i$. The von Neumann entropy is invariant under unitary transformations U , i. e., $S(U\sigma U^\dagger) = S(\sigma)$. Furthermore, if σ is a density matrix over a (finite-dimensional) Hilbert space \mathcal{H} , then $S(\sigma) \leq \log(\dim(\mathcal{H}))$. Finally, we formally introduce the kind of measurements that are relevant here.

Definition 6.4: Let J be a finite index set and let $\mathcal{M} = (P_i)_{i \in J}$ be a family of projection operators over the finite-dimensional Hilbert space \mathcal{H} with $\sum_{i \in J} P_i = I$. Then call \mathcal{M} a *projective measurement over \mathcal{H} with results in J* . For any density matrix σ over \mathcal{H} , define the *probability of measuring result $i \in J$ in the state described by σ* by $\Pr\{\mathcal{M}(\sigma) = i\} = \text{tr}(\sigma P_i)$.

The following lemma is due to Nayak. In the lemma, $H(p)$ denotes the binary entropy function defined by $H(p) = -p \log p - (1-p) \log(1-p)$.

Lemma 6.5 ([25]): Let σ_0 and σ_1 be density matrices over the finite-dimensional Hilbert space \mathcal{H} and let $\sigma = 1/2 \cdot (\sigma_0 + \sigma_1)$. Suppose there is a projective measurement $\mathcal{M} = (P_0, P_1)$ over \mathcal{H} with results in $\{0, 1\}$ such that for $b \in \{0, 1\}$, $\Pr\{\mathcal{M}(\sigma_b) = b\} \geq p \geq 1/2$. Then $S(\sigma) \geq (S(\sigma_0) + S(\sigma_1))/2 + (1 - H(p))$.

Now we are ready to prove the main result of this section, which is stated in the following theorem. The corollary directly follows from the upper bound on the OBDD size mentioned above.

Theorem 6.6: *The size of each QOBDD with bounded error for DISJ_n or IP_n is $2^{\Omega(n)}$.*

Corollary 6.7: $P\text{-OBDD} \not\subseteq BQP\text{-OBDD}$.

Proof of Theorem 6.6. We only prove the statement for disjointness, the claim for the inner product follows in the same way. Let a QOBDD G with some variable order π for DISJ_n be given. W.l.o.g. let G be leveled. Due to the symmetry of the OR-function, we may assume w.l.o.g. that for each $i \in \{1, \dots, n/2\}$ the variable x_{2i-1} is tested before x_{2i} in π . Let $p = 1/2 + \varepsilon$ be a lower bound on the success probability of G . We generate random inputs x for DISJ_n in the following way. Each variable with an odd index gets one of the values 0 and 1 with a probability of 1/2 each. All variables with an even index get the value 0. Let $\sigma(k)$ denote the density matrix describing the state of the QOBDD after reading the k th variable with an odd index. By induction we prove $S(\sigma(k)) \geq (1 - H(p))k$. Since the state of the QOBDD before reading the first randomly chosen variable is a pure state, we have $S(\sigma(0)) = 0$. Now let $k \geq 1$. By induction hypothesis $S(\sigma(k-1)) \geq (1 - H(p))(k-1)$. Let x_i be the k th variable with an odd index. Let U_0 and U_1 be the unitary transformations performed by the QOBDD while reading all the variables after the $(k-1)$ -st variable with an odd index and up to x_i inclusively, where the latter gets the value 0 or 1, resp. Since x_i is chosen to be 0 or 1 at random,

$$\sigma(k) = \frac{1}{2} \left(U_0 \sigma(k-1) U_0^\dagger + U_1 \sigma(k-1) U_1^\dagger \right).$$

Let U denote the composition of the unitary transformations performed by the QOBDD if the partner x_{i+1} of x_i gets the value 1 and all other variables read after x_i get the value 0. Then the function DISJ_n attains the value $c \in \{0, 1\}$ if $x_i = \bar{c}$. Let $\sigma = U\sigma(k)U^\dagger$. Since the QOBDD computes the function DISJ_n , the measurement of the QOBDD on σ yields the result c with a probability of at least p if x_i has the value \bar{c} . By Lemma 6.5 and the invariance of the von Neumann entropy under unitary transformations,

$$\begin{aligned} S(\sigma(k)) &= S(\sigma) \geq \frac{1}{2} \left(S(UU_0\sigma(k-1)U_0^\dagger U^\dagger) + S(UU_1\sigma(k-1)U_1^\dagger U^\dagger) \right) + 1 - H(p) \\ &\geq \frac{1}{2} (S(\sigma(k-1)) + S(\sigma(k-1))) + 1 - H(p). \end{aligned}$$

Then the claim follows by the induction hypothesis. We obtain the lower bound $(1 - H(p)) \cdot n/2$ on the von Neumann entropy of the density matrix describing the state of G after reading all variables with odd indices. By the above remark, this implies the lower bound $2^{(1-H(p)) \cdot n/2}$ on the dimension of the state space of G and, therefore, also on the size of G . \square

6.3. A Partial Function with Small QOBDDs that Requires Large Randomized OBDDs

An OBDD or QOBDD for a partially defined function has to compute the correct value of the function only on the domain of the function, while it may compute an arbitrary result on inputs outside the domain. We present a partially defined function with polynomial size QOBDDs but only exponential size randomized OBDDs. The idea behind the construction of the function is based on a result of Raz [31] for communication protocols.

The function we consider gets unitary matrices as inputs. In order to obtain a finitely representable function, we redundantly encode sufficiently precise approximations of the desired matrices by boolean variables. The redundancy in the encoding will allow us to prove a lower bound for arbitrary variable orders.

For the following, fix an even $n \in \mathbb{N}$ and let $\varepsilon > 0$. Let $b = 6(n-1)$ and let W_0, \dots, W_{b-1} be some fixed enumeration of the matrices in \mathcal{G}_n from Lemma 3.4. Let $k = k(n, \varepsilon) = O(n^2 \log(n/\varepsilon))$ be the number from this lemma. For $\ell \geq k$ and $m \geq b-1$ the *universal* (ε, ℓ, m) -code of $n \times n$ -matrices consists of the $\ell(m+1)$ boolean variables $x_{i,j}$, $1 \leq i \leq \ell$, $1 \leq j \leq m+1$. For $1 \leq i \leq \ell$ let $x_i = (x_{i,1}, \dots, x_{i,m+1})$ and $v(x_i) = x_{i,1} + \dots + x_{i,m}$. Let

$$U_i = \begin{cases} W_{(v(x_1) + \dots + v(x_i)) \bmod b}, & \text{if } x_{i,m+1} = 1; \\ I, & \text{if } x_{i,m+1} = 0. \end{cases}$$

Then the variable vector $x = (x_1, \dots, x_\ell)$ encodes the matrix

$$W(x) = U_\ell \cdot U_{\ell-1} \cdot \dots \cdot U_1.$$

Note that the variables $x_{i,m+1}$ only switch between $W_{(v(x_1) + \dots + v(x_i)) \bmod b}$ and the identity matrix. In particular, they do not influence the sum $(v(x_1) + \dots + v(x_i)) \bmod b$. By Lemma 3.4, for each unitary $n \times n$ -matrix U there is a setting to the x -variables such that $\|U - W(x)\| \leq \varepsilon$. In the following, ℓ is much larger than k such that there are many settings to obtain a certain unitary matrix in the product approximating U .

Now we define the considered function. Let $|1\rangle, \dots, |n\rangle$ be the standard basis of \mathbb{C}^n . Let V_0 and V_1 denote the subspaces spanned by the first and last $n/2$ of these basis vectors. Let $0 < \vartheta < 1/\sqrt{2}$. The input for the function $R_{\vartheta, \ell, m, n}$ consists of $3\ell(m+1)$ boolean variables $a_{i,j}, b_{i,j}, c_{i,j}, 1 \leq i \leq \ell, 1 \leq j \leq m+1$, which are interpreted as universal (ε, ℓ, m) -codes for three unitary $n \times n$ -matrices A, B, C , where $\varepsilon = 1/(3n)$. The function takes the value $z \in \{0, 1\}$ if the Euclidean distance between $CBA|1\rangle$ and V_z is at most ϑ . Otherwise the function is undefined.

We first prove the upper bound on the size of QOBDDs.

Theorem 6.8: *Let $0 < \vartheta < 1/\sqrt{2}$. The function $R_{\vartheta, 3k, 9kb, n}$ with an input size of $N = 81k^2b + 9k = O(n^5 \log^2 n)$ has QOBDDs with error at most ϑ^2 and size $O(N^{9/5}/\log^{8/5} N)$.*

Proof. Set $\ell = 3k$ and $m = 9kb$. We choose the variable order that starts with the a -variables ordered as $a_{1,1}, \dots, a_{1,m+1}, a_{2,1}, \dots, a_{2,m+1}, \dots, a_{\ell,1}, \dots, a_{\ell,m+1}$. Afterwards the b -variables and then the c -variables are tested in analogous orders. We first describe a subgraph G_A of the QOBDD evaluating the a -variables. Analogous subgraphs G_B and G_C are constructed for the b - and c -variables, resp.

The nodes of G_A are arranged in bn columns, which we label by (r, s) with $0 \leq r \leq b-1$ and $1 \leq s \leq n$, and in levels $1, \dots, \ell(m+1) + 1$. Let $|r\rangle|s\rangle|t\rangle$ be the vector from an orthonormal basis that corresponds to the node of the t th level in column (r, s) . The nodes in each of the first $\ell(m+1)$ levels are labeled by the same a -variable according to the variable order. The last level consists of sinks. Let $p \in \{1, \dots, \ell\}$. For $j \in \{1, \dots, m\}$, the node labeled by $a_{p,j}$ in column (r, s) is left by a single 0-edge with amplitude 1 leading to the node of the next level of the same column and a single 1-edge with amplitude 1 leading to the node of the next level in column $((r+1) \bmod b, s)$. For a node labeled by $a_{p,m+1}$ in column (r, s) , a single 0-edge with amplitude 1 leaving this node leads to the node in column (r, s) of the subsequent level. There are 1-edges connecting this node to the nodes of the subsequent level such that the mapping $|r\rangle|s\rangle|t\rangle \mapsto |r\rangle(W_r|s\rangle)|t+1\rangle$ is performed, where $t = (p-1)(m+1) + m + 1$.

It is easy to verify that the graph G_A constructed in this way is well-formed and unidirectional. We evaluate G_A according to the semantics of QBPs starting from a node on the first level in column (r, s) , i. e., with the superposition $|r\rangle|s\rangle|1\rangle$. Then after reading the variable vectors a_1, \dots, a_p , where $a_i = (a_{i,1}, \dots, a_{i,m+1})$, we reach the superposition $|r'\rangle(U_p \cdots U_1|s\rangle)|t\rangle$ with $r' = (r + v(a_1) + \dots + v(a_p)) \bmod b$ and $t = (p-1)(m+1) + m + 2$.

The QOBDD for $R_{\vartheta, \ell, m, n}$ starts with G_A , where the node on the first level in column $(0, 1)$ is chosen as the start node. Then the amplitude for reaching a node of the $(\ell(m+1) + 1)$ -st level in column (r, s) of G_A is exactly the s th coordinate of $A|1\rangle$, if r is the sum modulo b of all a -variables, and 0 otherwise. After reading the a -variables, the value of r is no longer needed; however, it cannot be erased in a QOBDD. Hence, for each possible value r we add a copy of a subgraph G_B processing the variables encoding B in the same way as described before for A . The sink in column (r, s) of the $(\ell(m+1) + 1)$ -st level of the subgraph G_A for A is identified with the node $(0, s)$ of the r th copy of the subgraph G_B for B . Altogether b copies of the subgraph G_B are sufficient. In the same way b^2 copies of a subgraph G_C for processing C are sufficient. In each copy of G_C , the sink in column (r, s) of the last level is a 0-sink if $s \leq n/2$, and a 1-sink otherwise. For each input, there is exactly one copy of G_C and exactly one r such that for all s the amplitude of the node in column (r, s) of the last level equals the s th coordinate of $CBA|1\rangle$. For all other copies of G_C and for all other r the amplitudes are 0.

Let E_z denote the projection to the subspace V_z . If $|y\rangle = CBA|1\rangle$ has distance at most ϑ from the subspace V_z , we have $\vartheta^2 \geq \||y\rangle - E_z|y\rangle\|^2 = 1 - \|E_z|y\rangle\|^2$. The equality follows by an easy calculation. Hence, the measurement on the level of the sinks leads to the result z

with probability $\|E_z|y\rangle\|^2 \geq 1 - \vartheta^2$. The size of the QOBDD is dominated by the b^2 copies of G_C . Each of these copies has size $O(bnN)$. Hence, the size can be estimated by $O(b^3nN) = O(n^9 \log^2 n) = O(N^{9/5} / \log^{8/5} N)$. \square

In order to prove the lower bound, we apply arguments from communication complexity (see, e.g., [16, 22] for an introduction). We first state a result of Raz [31], who has proved a lower bound on the communication complexity for a different function $R_{\vartheta,n}^0$. Using two rectangular reductions, which are defined below, we transfer this lower bound to a lower bound on the communication complexity of $R_{\vartheta,\ell,m,n}$ for any $\ell \geq k$ and $m \geq b-1$. Finally, by a standard lower bound technique for randomized OBDDs, the lower bound on the communication complexity implies a lower bound on the size of randomized OBDDs.

We define the function $R_{\vartheta,n}^0$ due to Raz by describing the corresponding communication problem. Let $0 < \vartheta < 1/\sqrt{2}$. The input of Alice consists of a unit vector $x \in \mathbb{R}^n$ and two orthogonal subspaces S_0 and S_1 of \mathbb{R}^n of dimension $n/2$ each. Bob gets an orthogonal real-valued $n \times n$ -matrix T as input. The output is $c \in \{0, 1\}$ if Tx has distance at most ϑ from S_c , and arbitrary otherwise. We remark that the usual definition of communication complexity can easily be extended to the case of infinite input sets which is considered here. Raz has proved the following result.

Theorem 6.9 ([31]): *Let $0 < \vartheta < 1/\sqrt{2}$. Each randomized communication protocol with bounded error for $R_{\vartheta,n}^0$ requires $\Omega(n^{1/2})$ bits of communication.*

We note that the considered communication problems are partially defined. On inputs for which such a problem is not defined, both outputs 0 and 1 are allowed. A partially defined communication problem on input sets X and Y can also be described by a relation $R \subseteq X \times Y \times \{0, 1\}$, where $(x, y, z) \in R$ iff z is a valid output for (x, y) . In particular, if the problem is undefined for (x, y) , we have $(x, y, 0), (x, y, 1) \in R$. A *rectangular reduction* from $R' \subseteq X' \times Y' \times \{0, 1\}$ to $R \subseteq X \times Y \times \{0, 1\}$ consists of two mappings $f: X' \rightarrow X$ and $g: Y' \rightarrow Y$ such that $(f(x), g(y), z) \in R \Rightarrow (x, y, z) \in R'$. It is easy to see that a lower bound on the communication complexity for R' implies the same lower bound for R if there is a rectangular reduction from R' to R .

We observe that the problem $R_{\vartheta,n}^0$ can easily be reduced to the following infinite precision variant $R'_{\vartheta,n}$ of the considered problem $R_{\vartheta,\ell,m,n}$. The input of $R'_{\vartheta,n}$ consists of unitary $n \times n$ -matrices A, B and C , where Alice gets A and C , and Bob gets B . Their task is to compute $z \in \{0, 1\}$ if the distance between $CBA|1\rangle$ and V_z is bounded by ϑ . (Again, $V_0 = \text{span}\{|1\rangle, \dots, |n/2\rangle\}$ and $V_1 = \text{span}\{|n/2+1\rangle, \dots, |n\rangle\}$.) Obviously, $R_{\vartheta,n}^0$ is a special case of $R'_{\vartheta,n}$. Instead of an orthogonal matrix T , a unitary matrix B is allowed. The vector x and the subspaces V_0 and V_1 are now encoded by the unitary matrices A and C . Hence, the lower bound from Theorem 6.9 also holds for $R'_{\vartheta,n}$. The second rectangular reduction is given in the following lemma.

Lemma 6.10: *For all constants ϑ, ϑ' with $0 \leq \vartheta' < \vartheta < 1/\sqrt{2}$, for all $\ell \geq k$ and $m \geq b-1$, and for sufficiently large n , $R'_{\vartheta',n}$ is reducible to $R_{\vartheta,\ell,m,n}$.*

Proof. Let (A', B', C') be an arbitrary input for $R'_{\vartheta',n}$. We map this input to an input for $R_{\vartheta,\ell,m,n}$ consisting of the universal (ε, ℓ, m) -codes of unitary $n \times n$ -matrices A, B, C with

$$\|A - A'\| \leq \varepsilon, \quad \|B - B'\| \leq \varepsilon, \quad \text{and} \quad \|C - C'\| \leq \varepsilon,$$

where $\varepsilon = 1/(3n)$. By Lemma 3.4, we can find such an input (A, B, C) for $R_{\vartheta,\ell,m,n}$. We show that this mapping is even a rectangular reduction. Let E_0 and E_1 be the projections on the subspaces V_0 and V_1 , resp. Let $|y\rangle = CBA|1\rangle$ and $|y'\rangle = C'B'A'|1\rangle$.

Let w.l.o.g. 0 be a solution of $R_{\vartheta,\ell,m,n}$ for the input (A, B, C) . Then either $\| |y\rangle - E_0|y\rangle \| \leq \vartheta$, i. e., the only valid output is 0, or $\| |y\rangle - E_0|y\rangle \| > \vartheta \wedge \| |y\rangle - E_1|y\rangle \| > \vartheta$, i. e., the outputs 0 and 1 are allowed. This is equivalent to $\| |y\rangle - E_1|y\rangle \| > \vartheta$. We prove that 0 is also a solution of the problem $R'_{\vartheta',n}$ for the input (A', B', C') by showing that $\| |y'\rangle - E_1|y'\rangle \| > \vartheta'$.

By the choice of A , B and C and by Proposition 3.6, we obtain $\| |y'\rangle - |y\rangle \| \leq 3\varepsilon = 1/n$. By the assumption, $\| E_0|y\rangle \| = \| |y\rangle - E_1|y\rangle \| > \vartheta$. Hence, $\| |y\rangle - E_0|y\rangle \| = (1 - \| E_0|y\rangle \|^2)^{1/2} < (1 - \vartheta^2)^{1/2}$ and thus

$$\| E_1|y'\rangle \| \leq \| E_1(|y'\rangle - |y\rangle) \| + \| E_1|y\rangle \| \leq \| |y'\rangle - |y\rangle \| + \| |y\rangle - E_0|y\rangle \| < \frac{1}{n} + (1 - \vartheta^2)^{1/2}.$$

This implies $\| |y'\rangle - E_1|y'\rangle \|^2 = 1 - \| E_1|y'\rangle \|^2 > \vartheta^2 - o(1)$. Since $\vartheta' < \vartheta$ and both ϑ, ϑ' are constants, it follows that $\| |y'\rangle - E_1|y'\rangle \| > \vartheta'$ for sufficiently large n . Hence, 0 is a solution of $R'_{\vartheta',n}$ for the input (A', B', C') . \square

Altogether we obtain a lower bound on the communication complexity of $R_{\vartheta,\ell,m,n}$ for $\ell \geq k$ and $m \geq b - 1$.

Corollary 6.11: *Let $0 < \vartheta < 1/\sqrt{2}$, $\ell \geq k$, and $m \geq b - 1$. Each randomized communication protocol with bounded error for $R_{\vartheta,\ell,m,n}$ where Alice has the matrices A and C and Bob the matrix B requires $\Omega(n^{1/2})$ bits of communication.*

Now we can prove the second part of the main result of this section, the lower bound on the size of randomized OBDDs with bounded error.

Theorem 6.12: *Let $0 < \vartheta < 1/\sqrt{2}$. Each randomized OBDD with bounded error for the function $R_{\vartheta,3k,9kb,n}$ on $N = 81k^2b + 9k = O(n^5 \log^2 n)$ variables has size $2^{\Omega(N^{1/10}/\log^{1/5} N)}$.*

It remains open to find an example of a *total* function with polynomial size QOBDDs but only exponential size randomized OBDDs. Using the currently available techniques, this seems to be difficult since the known lower bound techniques for randomized OBDDs, which are based on randomized communication complexity, also work in the quantum case (see Klauck [19]).

Proof of Theorem 6.12. Let G be a given randomized OBDD for $R_{\vartheta,\ell,m,n}$ with $\ell = 3k$ and $m = 9kb$ and with an arbitrary variable order. In general, the variables encoding the matrices A , B , and C do not occur as contiguous groups in the variable order. Because of the redundancy of the encoding of the matrices we can construct a suborder where the variables of each of the encodings of A , B , and C are grouped together such that the corresponding subproblem of $R_{\vartheta,\ell,m,n}$ is still hard. Then we can apply the above communication complexity lower bound. Let π denote the order of the variables $a_{i,j}, b_{i,j}, c_{i,j}$, $1 \leq i \leq \ell$, $1 \leq j \leq m$, in G . For A (and similarly B and C) call each set of variables $a_{i,1}, \dots, a_{i,m}$ in its encoding a *block*. The variables $a_{i,m+1}, b_{i,m+1}$, and $c_{i,m+1}$ do not occur in any block or in π .

Claim. *There is a suborder π' of π such that for each matrix of A , B and C there are exactly k consecutive blocks in π' that each contain exactly b variables.*

Proof of the claim. Think of π as a list of all variables (except $a_{i,m+1}, b_{i,m+1}$, and $c_{i,m+1}$) in the prescribed order. Observe that there are $9k$ blocks of $m = 9kb$ variables each encoding some matrix from the set \mathcal{G}_n .

We divide π into $9k$ contiguous parts such that for each block there is a part that contains at least b of its variables and such that for different blocks there are different parts with this property. The first of these parts is chosen by searching for the first position in the variable order π where for some block b variables have been tested (and hence for all other blocks less than b variables have been tested). Then this block is chosen and the other variables up to the chosen position are eliminated. Furthermore, all other variables of the chosen block are eliminated. An easy induction shows that this procedure can be iterated until $9k$ parts are chosen. Thus we are left with $9k$ smaller blocks with exactly b variables each and such that for each original block there is a smaller block in the list.

We now use the same idea to partition the list of variable blocks obtained in the first step into three parts such that for each of the three matrices there is a part containing at least k of its blocks and such that for different matrices there are different parts with this property. Again we eliminate variables in order to ensure that for each matrix exactly k consecutive blocks remain in the variable order. In this way, we obtain a variable order π' with the desired properties. \square

We replace all eliminated variables with 0 and remove the nodes labeled by these variables in the randomized OBDD and redirect incoming edges to the 0-successor. Furthermore, if all variables $a_{i,1}, \dots, a_{i,m}$ of a block are eliminated, we also replace $a_{i,m+1}$ with 0 and modify the randomized OBDD accordingly. The same is done for the eliminated blocks of b - and c -variables. This yields a randomized OBDD G' for $R_{\vartheta,k,b,n}$ that is at most as large as G .

We prove the desired lower bound for G' using the standard lower bound technique for randomized OBDDs (see, e. g., [42]). Observe that the variable order π' consists of three parts belonging to the different matrices A, B, C in some arbitrary order. Let C_1 be the set of nodes which are reached by some path on which exactly the variables for the first matrix according to π' have been tested, and let C_2 be the set of nodes which are reached by some path on which exactly the variables in the first two matrices have been tested. The OBDD can be used to build a randomized one- or two-round communication protocol for $R_{\vartheta,k,b,n}$ where Alice has the variables for A and C and Bob the variables for B . The players jointly follow a computation path in the OBDD from the start node to a sink, using random bits for decisions at random nodes of the OBDD and communicating the numbers of nodes in the sets C_1 and C_2 . The communication complexity of this protocol is bounded by $\lceil \log |C_1| \rceil + \lceil \log |C_2| \rceil \leq 2(\log |G'| + 1)$. Together with Corollary 6.11, this yields the claimed lower bound. \square

6.4. Las Vegas QOBDDs Versus Reversible OBDDs

The main result of this section is that $\text{ZQP-OBDD} \subseteq \text{Rev-OBDD}$. This means that even the zero-error QOBDD model with some failure probability is no more powerful with respect to polynomial size than reversible OBDDs.

The essence of the proof is as follows. Given a reversible OBDD G and a Las Vegas QOBDD G' for the same function and with the same variable order, we show that G' induces collections of measurements, called measurement schemes here, that allow to distinguish the subfunctions represented at each of the levels of G . We further prove that for such a measurement scheme, the dimension of the underlying Hilbert space can be lower bounded in terms of the number of those subfunctions. Altogether, we obtain a lower bound on the size of the Las Vegas QOBDD G' in terms of the size of the reversible OBDD G .

Definition 6.13: Let \mathcal{H} be a finite-dimensional Hilbert space and let $|v_1\rangle, \dots, |v_m\rangle \in \mathcal{H}$ be different pure quantum states. Let $X = \{1, \dots, m\}$ and $Y = \{1, \dots, n\}$. Call an $m \times n$ -matrix $A = (a_{ij})$ with entries in $\{0, 1, *\}$ and projective measurements $\mathcal{M}_j = (M_{j,0}, M_{j,1}, M_{j,?})$ with

possible results $\{0, 1, ?\}$, where $j = 1, \dots, n$, a *measurement scheme* for $|v_1\rangle, \dots, |v_m\rangle$ with zero error and failure probability ε , $0 \leq \varepsilon < 1$, if

- (i) for all different $i, j \in X$ there is a $k \in Y$ such that $a_{ik}, a_{jk} \in \{0, 1\}$ and $a_{ik} \neq a_{jk}$;
- (ii) for all $i \in X$ and $j \in Y$, if $a_{ij} = *$, then $a_{ik} = *$ for all $j \leq k \leq n$; and
- (iii) for all $i \in X$ and $j \in Y$, if $a_{ij} \in \{0, 1\}$, then $\Pr\{\mathcal{M}_j(|v_i\rangle) = a_{ij}\} \geq 1 - \varepsilon$ and $\Pr\{\mathcal{M}_j(|v_i\rangle) = \neg a_{ij}\} = 0$.

A measurement scheme allows us to distinguish any pair of vectors from $|v_1\rangle, \dots, |v_m\rangle \in \mathcal{H}$ by zero error measurements. Our aim is to prove a lower bound on the dimension of \mathcal{H} in terms of m . For this, we use the following lemma due to Klauck [19], which is a Las Vegas variant of Lemma 6.5.

Lemma 6.14 ([19]): *Let σ_0, σ_1 be density matrices over \mathcal{H} and let $0 \leq p \leq 1$. Suppose that there is a projective measurement $\mathcal{M} = (M_0, M_1, M_?)$ with possible results $\{0, 1, ?\}$ such that $\Pr\{\mathcal{M}(\sigma_b) = b\} \geq 1 - \varepsilon$ and $\Pr\{\mathcal{M}(\sigma_b) = \neg b\} = 0$ for all $b \in \{0, 1\}$. Let $\sigma = p\sigma_0 + (1 - p)\sigma_1$. Then $S(\sigma) \geq pS(\sigma_0) + (1 - p)S(\sigma_1) + (1 - \varepsilon)H(p)$.*

The following lemma extends a result of Klauck [19] that gives a lower bound on the Las Vegas one-way quantum communication complexity in terms of deterministic one-way communication complexity. The proof of Klauck provides the main idea of the proof of Lemma 6.15 for measurement schemes without “*”-entries.

Lemma 6.15: *Let $|v_1\rangle, \dots, |v_m\rangle \in \mathcal{H}$ be different pure quantum states. If there is a measurement scheme for $|v_1\rangle, \dots, |v_m\rangle$ with zero error and failure probability ε , then $\dim(\mathcal{H}) \geq m^{1-\varepsilon}$.*

Proof. Let A be the $m \times n$ -matrix with entries from $\{0, 1, *\}$, and let $\mathcal{M}_1, \dots, \mathcal{M}_n$ be the projective measurements in the given measurement scheme for $|v_1\rangle, \dots, |v_m\rangle$. Let $X = \{1, \dots, m\}$ and $Y = \{1, \dots, n\}$. Call two rows of a A *distinguishable* if they differ in a column where both of them have boolean values. Thus the rows of A are pairwise distinguishable according to the hypothesis.

In the following we inductively define a mixed state over \mathcal{H} with large von Neumann entropy in order to obtain the lower bound on the dimension of \mathcal{H} . The mixed states that we consider are convex combinations of the pure states $\sigma_i = |v_i\rangle\langle v_i|$, $i = 1, \dots, m$. For any $I \subseteq X$, $j \in Y$, and $b \in \{0, 1\}$ let $I_{j,b} = \{i \in I \mid a_{ij} = b\}$.

- (i) For $I \subseteq X$ with $|I| \geq 2$ and $j \in Y$ such that all rows in the submatrix $I \times \{j, j + 1, \dots, n\}$ of A are distinguishable, let $\sigma(I, j) = (|I_{j,1}|/|I|) \cdot \sigma(I_{j,1}, j + 1) + (|I_{j,0}|/|I|) \cdot \sigma(I_{j,0}, j + 1)$.
- (ii) Let $\sigma(\{i\}, j) = \sigma_i$ for $i \in X$ and $1 \leq j \leq n + 1$.

If the rows in the submatrix $I \times \{j, j + 1, \dots, n\}$ of A are distinguishable, by condition (ii) of Definition 6.13 the j th column of the submatrix only contains the entries 0 and 1: If it contained an entry “*”, the whole row would consist of “*” and would thus not be distinguishable from the other rows. It follows that $\sigma(X, 1)$ is well defined by a recursive application of the above definition, since (by induction), all rows in I are pairwise distinguishable as long as $|I| \geq 2$, in which case part (i) is applicable. After some applications of part (i), finally part (ii) is applicable.

Claim. *For each $I \subseteq X$ and $j \in Y$ such that all rows in the submatrix $I \times \{j, j + 1, \dots, n\}$ of A are distinguishable, $S(\sigma(I, j)) \geq (1 - \varepsilon) \log |I|$.*

By the claim $S(\sigma(X, 1)) \geq (1 - \varepsilon) \log m$ and $\dim(\mathcal{H}) \geq 2^{S(\sigma(X, 1))} \geq m^{1 - \varepsilon}$, which implies Lemma 6.15. It remains to prove the claim by an induction on the definition of $\sigma(I, j)$.

Induction base (Part (ii) of the definition): Then $S(\sigma(\{i\}, j)) = 0$ for all $i \in X$ and $1 \leq j \leq n + 1$.

Induction step (Part (i) of the definition): We consider $\sigma(I, j) = p \cdot \sigma(I_{j,0}, j + 1) + (1 - p) \cdot \sigma(I_{j,1}, j + 1)$, where $p = |I_{j,0}|/|I|$. Observe that $I = I_{j,0} \cup I_{j,1}$ and that for $b \in \{0, 1\}$, $\sigma(I_{j,b}, j + 1) = \sum_{i \in I_{j,b}} p_i \sigma_i$ for suitable probabilities p_i , $i \in I_{j,b}$, with $\sum_{i \in I_{j,b}} p_i = 1$ (the latter can also be proved by an easy induction on the definition of the $\sigma(I, j)$). Thus, applying the measurement \mathcal{M}_j to $\sigma(I_{j,b}, j + 1)$ yields

$$\Pr\{\mathcal{M}_j(\sigma(I_{j,b}, j + 1)) = b\} \geq 1 - \varepsilon \quad \text{and} \quad \Pr\{\mathcal{M}_j(\sigma(I_{j,b}, j + 1)) = \neg b\} = 0.$$

By Lemma 6.14, this implies

$$S(\sigma(I, j)) \geq p \cdot S(\sigma(I_{j,0}, j + 1)) + (1 - p) \cdot S(\sigma(I_{j,1}, j + 1)) + (1 - \varepsilon)H(p).$$

By the induction hypothesis, $S(\sigma(I_{j,b}, j + 1)) \geq (1 - \varepsilon) \log |I_{j,b}|$ for $b \in \{0, 1\}$. Thus,

$$\begin{aligned} S(\sigma(I, j)) &\geq p(1 - \varepsilon) \log |I_{j,0}| + (1 - p)(1 - \varepsilon) \log |I_{j,1}| + (1 - \varepsilon)H(p) \\ &= (1 - \varepsilon)(p \log |I_{j,0}| + (1 - p) \log |I_{j,1}| + H(p)). \end{aligned}$$

Using that $p|I| = |I_{j,0}|$ and $(1 - p)|I| = |I_{j,1}|$, we get

$$\begin{aligned} S(\sigma(I, j)) &\geq (1 - \varepsilon)(p \log(p|I|) + (1 - p) \log((1 - p)|I|) + H(p)) \\ &= (1 - \varepsilon)(p \log p + (1 - p) \log(1 - p) + H(p) + \log |I|) = (1 - \varepsilon) \log |I|, \end{aligned}$$

as desired. This completes the proof of the claim and thus the proof of Lemma 6.15. \square

Now we can state and prove the main result.

Theorem 6.16: *Let G be a minimum size, leveled, reversible π -OBDD for f . Let G' be a leveled π -QOBDD that computes f with zero error and failure probability ε , $0 \leq \varepsilon < 1$. For $i = 1, \dots, n + 1$, let L_i and L'_i be the sets of nodes on level i in G and G' , resp. Then $|L'_i| \geq |L_i|^{1 - \varepsilon}$ for $i = 1, \dots, n + 1$. In particular, $|G'| \geq |G|^{1 - \varepsilon}$.*

Corollary 6.17: *Rev-OBDD = EQP-OBDD = ZQP-OBDD.*

Proof of Theorem 6.16. W.l.o.g. let $G = (V, E)$ and $G' = (V', E')$ have the variable order x_1, \dots, x_n . From G and G' we construct some set of vectors which are intermediate states of the computation of G' . We exploit the relation to G in order to construct a measurement scheme for these vectors such that the lower bound follows from Lemma 6.15.

W. l. o. g. f depends on all variables. Let $\delta: V' \times V' \times \{0, 1\} \rightarrow \mathbb{C}$ denote the transition amplitudes of G' . Let \mathcal{H} be the Hilbert space spanned by an orthonormal basis $(|v\rangle)_{v \in V'}$ whose elements are identified with the nodes of G' . Let $s \in V$ and $s' \in V'$ be the start nodes of G and G' , resp., and let $F \subseteq V'$ be the set of sinks of G' . For a partial input assignment a to x_1, \dots, x_i , let $|\varphi(a)\rangle \in \mathcal{H}$ be the superposition reached in G' by carrying out its computation on a . Let $\mathcal{M}_{\text{sink}} = (M_{\text{sink},0}, M_{\text{sink},1}, M_{\text{sink},?})$ be the projective measurement of the output label at the sinks in G' . For $b \in \{0, 1\}$, fix a unitary operator U_b on \mathcal{H} such that $U_b|v\rangle = \sum_{w \in V'} \delta(v, w, b)|w\rangle$ for all $v \in V' - F$. Such an operator exists due to the well-formedness of G' .

By the assumptions of the theorem, L_i is the set of all nodes of G reached by partial assignments to x_1, \dots, x_{i-1} , for $i = 1, \dots, n+1$. Observe that $L_1 = \{s\}$ and, since G is leveled and f depends on all variables, all nodes in L_i , $1 \leq i \leq n$, are labeled by x_i . For a node $v \in V$, let f_v denote the subfunction of f represented at v according to the usual semantics of deterministic OBDDs.

We recursively construct mappings asn_i for $i = 1, \dots, n+1$ such that asn_i maps a node $v \in L_i$ to a partial assignment to x_1, \dots, x_{i-1} reaching that node from the start node of G . First, we choose $\text{asn}_1(s)$ as the empty assignment. Next consider a level L_i with $i > 1$. Let v_1, \dots, v_ℓ be all nodes representing one of the subfunctions f_{sub} represented at nodes in L_i . Since G is reversible and of minimum size, there are a constant $b \in \{0, 1\}$ and different nodes $u_1, \dots, u_\ell \in L_{i-1}$ such that $(f_{u_j})|_{x_{i-1}=b} = f_{\text{sub}}$ and there is a b -edge from u_j to v_j for $j = 1, \dots, \ell$. Define $\text{asn}_i(v_j) = (\text{asn}_{i-1}(u_j), b)$ for $j = 1, \dots, \ell$. For $i = 1, \dots, n+1$, let $C_i = \{|\varphi(\text{asn}_i(v))\rangle \mid v \in L_i\}$.

Claim. For each $i = 1, \dots, n+1$, there is a measurement scheme for C_i with zero error and failure probability ε .

By Lemma 6.15, the claim implies $|L'_i| \geq \dim(\text{span}(C_i)) \geq |L_i|^{1-\varepsilon}$ and thus the first part of the theorem. Since $(x_1 + \dots + x_k)^c \geq x_1^c + \dots + x_k^c$ for all $c \geq 1$ and $x_1, \dots, x_k \in \mathbb{R}_0^+$, also $|G'| \geq |G|^{1-\varepsilon}$ follows.

We prove the claim by induction on i . For $i = 1$ and $C_1 = \{|\varphi(\text{asn}_1(s))\rangle\} = \{|s'\rangle\}$ the empty measurement scheme has the required properties.

Let $i > 1$ and $L_i = \{v_1, \dots, v_m\}$. Let $Y = \{y_1, \dots, y_N\}$, $N = 2^{n-i+1}$, be the set of assignments to x_i, \dots, x_n . Define the $m \times N$ -matrix $A = (a_{jk})$ by setting $a_{jk} = f_{v_j}(y_k)$ for $1 \leq j \leq m$ and $1 \leq k \leq N$. For $k = 1, \dots, N$ let $\mathcal{M}_k = (M_{k,0}, M_{k,1}, M_{k,?})$ be the projective measurement with $M_{k,x} = M_{\text{sink},x} U_{y_k}$ where $x \in \{0, 1, ?\}$ and U_{y_k} is the unitary transformation carried out by G' for the partial input y_k when started on a superposition of the basis vectors $(|v\rangle)_{v \in L'_i}$.

Obviously, A is a boolean matrix where two rows $j, j' \in \{1, \dots, m\}$ differ iff the corresponding subfunctions f_{v_j} and $f_{v_{j'}}$ differ on an input from Y . Hence, for a each set of pairwise different rows of A chosen as representatives for the different subfunctions and vectors in C_i chosen accordingly, the above definitions yield a measurement scheme due to the fact that G' computes f with zero error and failure probability ε . Our goal is to extend the matrix A and the collection of measurements such that we obtain a measurement scheme for all vectors in C_i . We remark that A does not have entries “*”.

Consider a subset of rows of A belonging to the same subfunction f_{sub} and thus containing identical vectors. W.l.o.g., let v_1, \dots, v_ℓ be the respective nodes in L_i representing f_{sub} . Let $u_1, \dots, u_\ell \in L_{i-1}$ and $b \in \{0, 1\}$ be as in the definition of the assignments $\text{asn}_i(v_j)$ above. In particular, b is the same constant for u_1, \dots, u_ℓ . Then $U_b |\varphi(\text{asn}_{i-1}(u_j))\rangle = |\varphi(\text{asn}_{i-1}(u_j), b)\rangle = |\varphi(\text{asn}_i(v_j))\rangle$. By induction hypothesis, there is measurement scheme for C_{i-1} . Let D be the matrix of this measurement scheme, which is of size $|C_{i-1}| \times p$ for some p . Consider the subscheme for the vectors $|\varphi(\text{asn}_{i-1}(u_j))\rangle$, $j = 1, \dots, \ell$, which we obtain from D by deleting the rows corresponding to the other vectors. Let this measurement scheme be described by the $\ell \times p$ -matrix $B = (b_{jk})$ and the projective measurements $\mathcal{P}_k = (P_{k,0}, P_{k,1}, P_{k,?})$, $k = 1, \dots, p$. Define $\mathcal{P}'_k = (P'_{k,0}, P'_{k,1}, P'_{k,?})$, $k = 1, \dots, \ell$, by $P'_{k,x} = P_{k,x} U_b^\dagger$ for $x \in \{0, 1, ?\}$.

Then for $j \in \{1, \dots, \ell\}$ and $k \in \{1, \dots, p\}$ such that $b_{jk} \in \{0, 1\}$,

$$\begin{aligned} \Pr\{\mathcal{P}'_k(|\varphi(\text{asn}_i(v_j))\rangle) = b_{jk}\} &= \|P'_{k,b_{jk}} |\varphi(\text{asn}_i(v_j))\rangle\|^2 = \|P_{k,b_{jk}} U_b^\dagger |\varphi(\text{asn}_i(v_j))\rangle\|^2 \\ &= \|P_{k,b_{jk}} U_b^\dagger U_b |\varphi(\text{asn}_{i-1}(u_j))\rangle\|^2 \\ &= \Pr\{\mathcal{P}_k(|\varphi(\text{asn}_{i-1}(u_j))\rangle) = b_{jk}\}. \end{aligned}$$

Hence, the measurements \mathcal{P}'_k , $k = 1, \dots, p$, satisfy property (iii) in the definition of measurement schemes with respect to the matrix B .

Let B_1, \dots, B_R be all submatrices of D obtained by the above construction for the different subfunctions of f_v , $v \in L_i$. Since in the construction of B_1, \dots, B_R no columns of D are deleted, the columns of B_1, \dots, B_R are labeled by the same measurements. Hence, we can attach the matrices B_1, \dots, B_R to A as submatrices in the columns $m + 1, \dots, m + p$ and fill up the remaining entries with “*” such that the new matrix A' obtained in this way and the measurements $\mathcal{M}_1, \dots, \mathcal{M}_N, \mathcal{P}'_1, \dots, \mathcal{P}'_p$ comprise a measurement scheme for C_i with zero error and failure probability ε . Since A does not have any “*”-entries, also property (ii) of Definition 6.13 is fulfilled. \square

The above lower bound on the size of zero error QOBDDs in terms of the size of reversible OBDDs is essentially optimal, as the following example shows. For $n = 2^\ell$ define the *index function* $\text{IND}_n: \{0, 1\}^{n+\ell} \rightarrow \{0, 1\}$ on variable vectors $x = (x_0, \dots, x_{n-1})$ and $y = (y_0, \dots, y_{\ell-1})$ by $\text{IND}_n(x, y) = x_{|y|}$, where $|y| = \sum_{i=0}^{\ell-1} y_i 2^i$.

Proposition 6.18: *For the variable order π described by $(x_0, \dots, x_{n-1}, y_0, \dots, y_{\ell-1})$, each deterministic π -OBDD representing IND_n requires size 2^n , while the same function can be computed by zero error π -QOBDDs with failure probability ε of size $2^{(1-\varepsilon)n+O(\log n)}$.*

Hromkovič and Schnitger [17] have used a similar function to prove an analogous result for classical Las Vegas and deterministic one-way communication complexity and the special case of failure probability $\varepsilon = 1/2$. The proof of the proposition is by a straightforward adaptation of a simple randomized OBDD to the quantum case.

Proof. The lower bound for deterministic OBDDs is well known and follows from the fact that IND_n has maximal one-way communication complexity with respect to the partition of variables where Alice obtains x and Bob obtains y . In the following, we briefly sketch the upper bound construction.

For $\varepsilon \geq 1/2$, partition x into $k = \lfloor 1/(1-\varepsilon) \rfloor$ blocks of size approximately $(1-\varepsilon)n$. The QOBDD chooses one of these blocks at random by an unlabeled node at the top (which can be removed later on similarly to the proof of Theorem 6.2) with outgoing edges having amplitudes $1/\sqrt{k}$. These edges lead to sub-QOBDDs where the complete chosen block is read and stored, which requires a binary tree with $O(2^{(1-\varepsilon)n})$ nodes for each block. At each leaf of such a tree, append a tree of size $O(n)$ reading y and computing $|y|$. Finally, a sink with the correct output value is reached if $|y|$ lies in the chosen block, which happens with probability at least $1/k \geq 1-\varepsilon$. Otherwise, the “?”-sink is reached.

For $\varepsilon < 1/2$, we select $k = \lceil 1/\varepsilon \rceil$ blocks of x -variables of size approximately $(1-\varepsilon)n$ that cover each single variable exactly $k-1$ times. The rest of the construction is the same as above. The failure probability is obviously bounded above by $1/k \leq \varepsilon$. \square

6.5. Comparison of QOBDDs and Read-Once QBPs

In this section we observe that, similarly to the classical case, QOBDDs are a more restricted model of QBPs than read-once QBPs. A function separating these two models with respect to polynomial size is the so-called *indirect storage access function*, which is defined in the following way. Let $n = 2^k$. The input of ISA_n consists of the variables y_0, \dots, y_{k-1} and x_0, \dots, x_{n-1} . The y -variables are interpreted as a binary number s . The x -variables are partitioned into $b = \lfloor n/k \rfloor$ blocks of size $k = \log n$, which are numbered beginning with 0. If $s \geq b$, the output

is 0. Otherwise the s th block is again interpreted as a binary number t and the output is x_t . It is straightforward to construct a decision tree for ISA_n of size $O(n^2/\log n)$, which can also be regarded as a read-once QBP.

The lower bound for QOBDDs for all variable orders is a straightforward combination of two results. Klauck [19] proved the lower bound $\Omega(n)$ on the quantum one-way communication complexity of IND_n , where Alice gets the x -variables and Bob the y -variables. This lower bound directly implies the lower bound $2^{\Omega(n)}$ on the size QOBDDs for IND_n , where the x -variables are tested before the y -variables. Using a rectangular reduction, it has been shown in [34] that an OBDD for ISA_n and an arbitrary variable order cannot be smaller than an OBDD for $\text{IND}_{\lfloor n/\log n \rfloor - 1}$ and the variable order mentioned before. This also holds for QOBDDs such that we obtain the lower bound $2^{\Omega(n/\log n)}$ on the size for QOBDDs for ISA_n and an arbitrary variable order.

7. QBPs with Generalized Measurements

The usual unitary quantum mode of computation has turned out to be only of limited use for such restricted models as quantum OBDDs and quantum finite automata. In this section we consider a generalization of QBPs where in each step the performed unitary operation is determined by the result of a previous measurement. We first present the definition of QBPs with generalized measurements and we discuss the relationship to QBPs and to randomized BPs. Afterwards, we prove a generic lower bound on the size of QOBDDs with generalized measurements for so-called k -stable functions.

Definition 7.1: Let $k \in \mathbb{N}$ with $k \geq 3$. A *quantum branching program with generalized measurements (gmQBP)* over the variable set $X = \{x_1, \dots, x_n\}$ is a directed multigraph $G = (V, E)$ with a start node $s \in V$, a set of sinks $F \subseteq V$, and transition amplitudes δ . Nodes and edges are labeled in the same way as in a usual QBP (see Definition 2.4). Additionally, there is a partition $(V_0, V_1, V_2, \dots, V_{k-1})$ of V such that V_0 and V_1 consist of the 0- and 1-sinks of G , resp. The edge labels of the gmQBP G have to fulfill the following modified well-formedness constraint. Let $u, v \in V_\ell$, $\ell \in \{2, \dots, k-1\}$, be interior nodes with $\text{var}(u) = i$ and $\text{var}(v) = j$, resp. Then for all assignments $a = (a_1, \dots, a_n)$ to the variables in X ,

$$\sum_{w \in V} \delta^*(u, w, a_i) \delta(v, w, a_j) = \begin{cases} 1, & \text{if } u = v; \\ 0, & \text{otherwise.} \end{cases} \quad (\text{W}^*)$$

Furthermore, gmQBPs are unidirectional, i. e., for each $w \in V$, all $v \in V$ for which a $b \in \{0, 1\}$ exists such that $\delta(v, w, b) \neq 0$ are labeled by the same variable.

We remark that the well-formedness condition for gmQBPs is weaker than the well-formedness condition for ordinary QBPs, because it has only to hold for pairs of nodes of the same set V_ℓ .

We now define the semantics of gmQBPs. As in the definition of usual QBPs, nodes correspond to vectors in an orthonormal basis $(|v\rangle)_{v \in V}$ of $\mathcal{H} = \mathbb{C}^{|V|}$ and intermediate results of the computation are superpositions of these vectors. As for QBPs, a computation step consists of a measurement and the subsequent transition to successor nodes according to the transition amplitudes δ . In a gmQBP, the measurement generalizes that allowed for QBPs as follows. The gmQBP performs the projective measurement $\mathcal{M} = (P_0, P_1, P_2, \dots, P_{k-1})$ with results $\{0, 1, 2, \dots, k-1\}$, where

$$P_r = \sum_{v \in V_r} |v\rangle\langle v|, \quad r \in \{0, 1, 2, \dots, k-1\}.$$

The probability of obtaining the result r is $\|P_r|\psi\rangle\|^2$. If the result r is 0 or 1, the computation stops with output r . If $r \geq 2$, the computation continues with the normalized projection

$$|\psi'\rangle = \frac{P_r|\psi\rangle}{\|P_r|\psi\rangle\|} = \sum_{v \in V_r} \alpha_v |v\rangle.$$

Then for each node $v \in V_r$ with $\text{var}(v) = i$ the gmQBP follows the edges with boolean label a_i according to their amplitudes. This yields the new superposition

$$|\psi''\rangle = \sum_{v \in V_r} \alpha_v \sum_{w \in V} \delta(v, w, a_{\text{var}(v)}) |w\rangle.$$

The above definition does not allow “?” outputs for simplicity, since we do not consider Las Vegas gmQBPs, anyway. The modified well-formedness constraint implies that for each result of the measurement the corresponding mapping can be extended to a unitary transformation. Computation time and acceptance modes are defined analogously to QBPs. Also the definition of QOBDDs with generalized measurements (gmQOBDDs) is straightforward: The variables are required to be tested according to a fixed variable order. We remark that gmQBPs have a simple graphic representation. Additionally to the representation of QBPs there is merely a partition of the nodes.

The physical realizability of gmQBPs depends on the ability to perform measurements during a computation. Based on a standard argument using Neumark’s theorem (see, e.g., [29]), such measurements can be described by unitary transformations in an extended Hilbert space. Furthermore, intermediate measurements are also possible, e.g., in the quantum circuit model defined in the textbook of Nielsen and Chuang [26] as well as in the model of Aharonov, Kitaev and Nisan [4] which allows gates computing general quantum operations (superoperators).

It is obvious that a QBP is a gmQBP with three possible measurement results. We show that randomized BPs can easily be transformed into gmQBPs.

Proposition 7.2: *For each randomized BP G computing some function f there is a gmQBP G' computing the same function with the same acceptance mode, and the size of G' is bounded above by the size of G .*

Proof. We remove all randomized nodes from G by allowing each node to have several outgoing 0- and 1-edges labeled by appropriate probabilities. In the corresponding gmQBP there are the same edges, where the probability p is replaced with the amplitude \sqrt{p} . The partition of the node set consists of the set of 0-sinks, the set of 1-sinks and sets each containing exactly one interior node. An easy induction shows that for each input the acceptance probabilities of G and G' coincide. \square

With the currently available techniques we cannot prove superpolynomial lower bounds for BPs and for QBPs either (cf. Proposition 2.7). Thus we are not able to prove that polynomial size gmQBPs are more powerful than polynomial size QBPs. However, for QOBDDs this is easy, even for $k = 4$, i.e., the smallest k where gmQOBDDs are a generalization of QOBDDs. In Theorem 6.6 we have proved exponential lower bounds on the size of QOBDDs for the function DISJ and IP. On the other hand, it is easy to construct linear size deterministic OBDDs for DISJ and IP. A careful inspection shows that each node of these OBDDs has at most two incoming 0-edges and at most one incoming 1-edge. We partition the internal nodes into two sets V_2 and V_3 such that each pair of nodes with the same 0-successor is not in the same set. Furthermore, by duplicating the sinks we ensure that each sink has at most one predecessor. The sets V_0 and V_1 are the sets of 0- and 1-sinks, resp., that are obtained in this way. We obtain the following result.

Proposition 7.3: *There are gmQOBDDs of linear size with $k = 4$ possible measurement results that exactly compute DISJ_n and IP_n .*

Finally, we prove a generic lower bound on the size of gmQOBDDs for k -stable functions. A function $f: \{0, 1\}^n \rightarrow \{0, 1\}$ is called k -stable if for each set V of variables of size k and each variable $x_i \in V$ there is a setting of the variables outside V such that the resulting subfunction is x_i or \bar{x}_i . It is well known that k -stable functions only have read-once branching programs of size 2^{k-1} , and it has been shown in [34] that also randomized OBDDs require size $2^{\Omega(k)}$. Examples for such functions include the determinant of an $n \times n$ -matrix over \mathbb{Z}_2 , which is $(n - 1)$ -stable, and the function checking whether a graph on n vertices has an $n/2$ -clique, which is $(n/4 + 1)$ -stable. For these and other examples, see Wegener [42].

We remark that the state of a gmQOBDD after performing a measurement during a computation can be described as a mixed state, i. e., a probability distribution over pure states. Now we can apply a lower bound on the quantum communication complexity for the index function (defined at the end of Section 6.4) due to Klauck [19].

Theorem 7.4: *Each gmQOBDD with bounded error for a k -stable functions has size $2^{\Omega(k)}$.*

Proof. W.l.o.g. let $k = 2^\ell$. Klauck [19] has observed that the quantum one-way communication complexity of the function IND_k is lower bounded by $\Omega(k)$ for the partition where the first player Alice gets the input vector $x = (x_0, \dots, x_{k-1})$ and the second player Bob gets $y = (y_0, \dots, y_{\ell-1})$. This lower bound also holds for the two-sided error model and if Alice may send a mixed state to Bob. Let a gmQOBDD for a k -stable function f be given. Then IND_k can be computed by a quantum one-way protocol in the following way: Alice may choose the first k variables in the variable order and Bob the remaining variables. By the property of k -stable functions, for each of Alice's variables, Bob can fix his variables such that the gmQOBDD outputs the value of the variable or its complement. Hence, it suffices for Alice to perform the computation of the gmQOBDDs of the first k levels for the given setting of her x -variables and to send the (mixed) state of the gmQOBDD after her computation to Bob. Bob can then compute the output as described. The communication complexity is bounded above by the logarithm of the size (or even the width) of the gmQOBDD. Together with the lower bound on the quantum communication complexity for IND_k , the theorem follows. \square

8. Open Problems

In this paper, we have explored the foundations of space-bounded nonuniform quantum complexity to some extent, but several interesting problems nevertheless remain open.

- It is not clear whether algebraic amplitudes for nonuniform QTMs and short amplitudes for QBPs are the most general reasonable sets of amplitudes. Is it possible to provide some formal argument that excludes more general sets of amplitudes (as done by Adleman, DeMarras, and Huang [3] for the uniform case and arbitrary complex amplitudes)?
- For space-bounded nonuniform QTMs with algebraic amplitudes we have proved that the general model can be simulated by the unidirectional one. It is open so far whether an analogous simulation also exists for the uniform case. Furthermore, for QBPs it is straightforward to define a variant without the requirement of unidirectionality. Can this generalized model be simulated by the unidirectional model or is it unreasonably powerful?

- It remains open whether there is a space-efficient simulation of QBPs by nonuniform QTMs for the cases of error-free and exact quantum computation and, if not, to provide some evidence showing that such a simulation is unlikely to exist.
- With respect to the comparison of OBDDs and QOBDDs, the relationship between the classes BQP-OBDD and BPP-OBDD for total functions is left open.
- Prove lower bounds for more general variants of QBPs. While lower bounds for QOBDDs can be obtained using tools from quantum communication complexity, already the proof of lower bounds for (possibly unordered) read-once QBPs seems to require new arguments.
- The model of gmQBPs remains largely open to investigation. In particular, the relationship between the standard model of QBPs and gmQBPs needs to be further clarified. Show separation results as that for QOBDDs and gmQOBDDs presented here also for more general variants of QBPs or investigate simulations of gmQBPs by usual QBPs.

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