Quantum Optimization Problems

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Abstract. Krentel [J. Comput. System Sci., 36, pp.490–509] presented a framework for an NP optimization problem that searches an optimal value among exponentially-many outcomes of polynomial-time computations. This paper expands his framework to a quantum optimization problem using polynomial-time quantum computations and introduces the notion of an “universal” quantum optimization problem similar to a classical “complete” optimization problem. We exhibit a canonical quantum optimization problem that is universal for the class of polynomial-time quantum optimization problems. We show in a certain relativized world that all quantum optimization problems cannot be approximated closely by quantum polynomial-time computations. We also study the complexity of quantum optimization problems in connection to well-known complexity classes.

Keywords: optimization problem, quantum Turing machine, universal problems

1 Introduction

Quantum computation theory was initiated in the early 1980s and has shown significant phenomena beyond the classical framework. During the 1990s, many classical concepts in complexity theory were examined and interpreted in quantum context, including the notions of “bounded-error polynomial-time computation” [1], “interactive proof system” [28], “parallel query computation” [33, 6], “Kolmogorov complexity” [27, 5], and “Merlin-Arthur game” [29, 18]. Along this line of research, this paper studies a quantum interpretation of a classical optimization problem.

An optimization problem is in general a certain type of search problem which is to find, among candidates to which some values are assigned, the maximal (or minimal) value or to find a solution with such the value. A typical example of such an optimization problem is the traveling salesperson problem that asks, upon given a map of cities and their traveling distances, for the length of a shortest tour to all the cities in the map. In the 1980s, Krentel [20] laid out a framework for studying the complexity of such optimization problems. He defined $\text{OptP}$ to be the collection of functions outputting the maximal (or minimal) value of indexed functions computable in polynomial-time. To locate the hardest optimization problems in $\text{OptP}$, Krentel introduced the notion of “completeness” under his metric reduction. The Traveling Salesperson Problem turns out to be a complete optimization problem for $\text{OptP}$ [20].

This paper studies a quantum interpretation of Krentel’s optimization problem. Krentel’s framework is easily generalized to the problem of optimizing the acceptance probability of indexed polynomial-time quantum computations. In consistence with Krentel’s notation, the notation $\text{Opt}\#\text{QP}$ is used for the class of these problems. However, this is a mixture of classical indexing and quantum computations. Instead, we introduce quantum functions indexed with a quantum state of polynomially-many qubits (called a quantum index). A quantum optimization problem, discussed in this paper, is to ask for a maximal acceptance probability of quantum computations labeled with quantum indices. We use the notation $\text{Qopt}\#\text{QP}$ to denote the collection of such quantum optimization problems.

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†The collection of all functions that output the acceptance probability of certain polynomial-time well-formed Turing machines is denoted $\#\text{QP}$ in [33].
These quantum optimization problems are also characterized by maximal eigenvalues of certain types of positive semidefinite, contractive, Hermitian matrices. In Section 4, we use this characterization to show fundamental properties of quantum optimization problems in $\text{Qopt} \# \text{QP}$.

The existence of complete optimization problems has largely contributed to the success of the theory of NP optimization problems. These complete optimization problems are considered, among all NP optimization problems, as the “hardest” problems to solve. In Section 5, we develop a similar “hardest” notion for quantum optimization problems. As shown by Bernstein and Vazirani [3], there exists a universal quantum Turing machine that simulates any well-formed quantum Turing machine with amplitudes approximable in polynomial time at the cost of polynomial slowdown. Different from a classical universal Turing machine, since all amplitudes are only approximated, the universal quantum Turing machine can simulate other machines only approximately to within a given closeness parameter. This manner of simulation gives rise to the notion of approximate reduction. We say that a function $f$ is approximately reducible to another function $g$ if $f$ has a Krentel’s metric-type reduction from $f$ to a certain function that approximates $g$ to within $1/m$, where $m$ is an accuracy parameter given as an auxiliary input to the reduction. In this fashion, we can define the notion of universal optimization problems for the class $\text{Qopt} \# \text{QP}$. This notion requires two functions to be apart only in a distance that is a reciprocal of a polynomial. In Section 6, we exhibit an example of a canonical universal optimization problem, which can be viewed as a generalization of the Bounded Halting Problem for NP. This notion of universality naturally induces promise-complete problems for many well-known quantum complexity classes, such as $\text{BQP}$ and $\text{QMA}$, which are believed to lack complete problems.

The class $\text{Qopt} \# \text{QP}$ includes its underlying class $\# \text{QP}$ as well as $\text{Opt} \# \text{QP}$. However, the complexity of $\text{Qopt} \# \text{QP}$ is not well-understood even in comparison with $\# \text{QP}$. This function class $\text{Qopt} \# \text{QP}$ naturally introduces the class of decision problems $\text{QOP}$ (“quantum optimization polynomial time”) in such a way that $\text{PP}$ is characterized by two $\# \text{P}$-functions. This class $\text{QOP}$ lies between $\text{PP}$ and $\text{PSPACE}$. In Section 7, we show that, under the assumption $\text{EQP} = \text{QP}$, every quantum optimization problem in $\text{Qopt} \# \text{QP}$ can be closely approximated by functions in $\# \text{QP}$. We may not remove the assumption because there exists a counterexample in a relativized world. Moreover, if every quantum optimization problem in $\text{Qopt} \# \text{QP}$ can be closely approximated by functions in $\# \text{QP}$, then $\text{QOP}$ is included in $\text{P} \# \text{P}$

The quantum optimization problems are also used to characterize other major complexity classes. One of the useful tools is the notion of “definability”, which is adapted from an earlier work of Fenner et al. [1]. A complexity class $\mathcal{C}$ is called $\text{Qopt} \# \text{QP}$-definable if we have a pair of disjoint sets $A, R \subseteq \Sigma^* \times \mathbb{R}$ such that every set $A$ in $\mathcal{C}$ has witnesses $f$ in $\text{Qopt} \# \text{QP}$; that is, for every $x$, if $x \in A$ then $(x, f(x)) \in A$ and otherwise $(x, f(x)) \in R$. An obvious example of such $\text{Qopt} \# \text{QP}$-definable sets is the class $\text{QMA}$, a quantum version of Merlin-Arthur proof systems [13, 23, 28]. A less trivial example is $\text{NQP}$, introduced by Adleman et al. [9]. However, it is not yet known whether $\text{PP}$ is $\text{Qopt} \# \text{QP}$-definable. We present a partial answer to this question in Section 8 by giving a new characterization of $\text{PP}$ in terms of quantum optimization problems. This characterization also yields Watrous’s recent result that $\text{QMA}$ is included in $\text{PP}$ [10].

The $\text{Qopt} \# \text{QP}$-definability gives light to the relationship between $\text{Qopt} \# \text{QP}$ and other well-known complexity classes. From a different perspective, we focus on the structure of the complexity classes that are induced from $\text{Qopt} \# \text{QP}$. An example of such complexity classes is the class $\text{QOP}$. Based upon our new characterization of $\text{PP}$ in Section 5, we introduce the new complexity class $\text{AQMA}$. In Section 9, we first show several Boolean closure properties of $\text{QOP}$ and $\text{AQMA}$. Another important concept in complexity theory is low sets. Any set $A$ that bears only poor information when it is used as an oracle for relativizable class $\mathcal{F}$ (that is, $\mathcal{F}^A = \mathcal{F}$) is called an $\mathcal{F}$-low set. We show

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‡ A set $S$ is in $\text{PP}$ iff there exit two functions $f, g \in \# \text{P}$ such that, for every $x, x \in A \Leftrightarrow f(x) > g(x)$. 

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that the class of $\mathsf{Qopt}$-$\#\mathsf{QP}$-low sets lies between $\mathsf{EQP}$ and $\mathsf{EQMA}$, which is an error-free version of $\mathsf{QMA}$ \cite{4}. This contrasts the known result that the class of $\#\mathsf{QP}$-low sets is exactly $\mathsf{EQP}$ \cite{5}.

2 Preliminaries

We introduce important notions and notation in this section.

Let $\mathbb{N}$, $\mathbb{R}$, and $\mathbb{C}$ denote the sets of all natural numbers (e.g., nonnegative integers), of all real numbers, and of all complex numbers, respectively. Let $\mathbb{N}^+ = \mathbb{N} \setminus \{0\}$. Let $\mathbb{D}$ be the collection of all dyadic rational numbers, where a dyadic rational number is of the form $0.r$ or $-0.r$ for a certain finite series $r$ of 0s and 1s. In this paper, a polynomial means a multi-variate polynomial with nonnegative integer coefficients.

For any function $f$ and any integer $m > 0$, $f^m$ denotes the function satisfying $f^m(x) = (f(x))^m$ for all $x$. For example, $\log^k n$ means $(\log n)^k$ for each $k \in \mathbb{N}^+$. The notation $A^B$, where $A$ and $B$ are any nonempty sets, denotes the set of all total functions mapping from $A$ to $B$: for example, $\mathbb{N}^\mathbb{N}$, $\mathbb{D}^\mathbb{N}$, etc. For any two functions $f$ and $g$ with the same domain, we say that $f$ majorizes $g$ if $f(x) \geq g(x)$ for all $x$ in the domain of $g$.

Any element of a Hilbert space (i.e., a complex vector space with the standard inner product) of finite dimension is expressed by Dirac’s ket notation $|\cdot\rangle$. For an $n \times n$ matrix $A = (a_{ij})_{1 \leq i,j \leq n}$ over $\mathbb{C}$, the notation $A^\dagger$ denotes the Hermitian adjoint (i.e., the transposed complex conjugate) of $A$. Moreover, $\|A\|$ denotes the operator norm of $A$ defined by $\sup\{\|A|\phi|\|/\|\phi\|\}$, where the supremum is over all nonzero vectors $|\phi\rangle$. Note that if $A$ is Hermitian, then $\|A\| = \sup_{|\phi\rangle \neq 0} \{|\langle A|\phi|\rangle/\|\phi\|\|\}$. A square matrix $A$ is contractive if $\|A\| \leq 1$. See, e.g., \cite{6} for more detail.

Classical Complexity: Our alphabet is $\Sigma = \{0,1\}$ throughout this paper and assume the standard (canonical and lexicographical) order on $\Sigma^*$. The empty string is denoted $\lambda$. For a string $x$, $|x|$ denotes the length of $x$. We assume the reader’s familiarity with multi-tape, off-line Turing machines (TMs).

We fix a pairing function $(\cdot,\cdot)$, which is a one-to-one map from $\Sigma^* \times \Sigma^*$ to $\Sigma^*$, satisfying that, for a certain polynomial $p$, $|\langle x,y \rangle| \leq p(|x|,|y|)$ for all $x$ and $y$. In particular, we assume that the paring function preserves the length, that is, $|\langle x,y \rangle| = |\langle x',y' \rangle|$ whenever $|x| = |x'|$ and $|y| = |y'|$.

Let $\mathcal{C}$ be the set of all polynomial-time approximable complex numbers (that is, the real and imaginary parts are approximated to within $2^{-k}$ in time polynomial in the size of input together with $k$). For any two sets $A$ and $B$, $A \oplus B$ is the disjoint union of $A$ and $B$ defined by $A \oplus B = \{0x \mid x \in A\} \cup \{1x \mid x \in B\}$.

We also assume the reader’s familiarity with basic complexity classes: $\mathsf{P}$, $\mathsf{NP}$, co-$\mathsf{NP}$, $\mathsf{BPP}$, $\mathsf{PP}$, $\mathsf{PSPACE}$, and $\mathsf{EXP}$. The definition of theses complexity classes are found in, e.g., \cite{7} [14]. In particular, we use the notation $\mathsf{FP}$ to denote the collection of all polynomial-time computable functions from $\Sigma^*$ to $\Sigma^*$. Similarly, $\mathsf{FPSPACE}$ is defined as the collection of polynomial-space computable functions whose outputs are also bounded by polynomials.

The class $\#\mathsf{P}$ consists of all functions $f$ from $\Sigma^*$ to $\mathbb{N}$ whose values are exactly the number of accepting paths of some polynomial-time nondeterministic TMs \cite{16}. Moreover, $\mathsf{GapP}$ is the set of functions from $\Sigma^*$ to $\mathbb{Z}$ that calculate the difference between the number of accepting paths and the number of rejecting paths of polynomial-time nondeterministic TMs \cite{14}. For convenience, we translate the binary outcome of a Turing machine to an integer or a dyadic rational number by identifying $\{0,1\}^*$ with $\mathbb{Z}$ or $\{\pm 0.r \mid r \in \{0,1\}^*\}$ in the standard order. By this identification, we have the basic inclusions: $\mathsf{FP} \subseteq \#\mathsf{P} \subseteq \mathsf{GapP} \subseteq \mathsf{FPSPACE}$.

\footnote{To translate an integer or a dyadic rational number into a string, we use the first bit (called the sign bit) of the string to express the sign (that is, + or –) of the number.}
Quantum Complexity: A quantum state is a vector of unit norm in a Hilbert space. A quantum bit (qubit, for short) is a quantum state of two-dimensional Hilbert space. We mainly use the standard basis \{0, 1\} to express a quantum state. Any quantum state in 2^n-dimensional Hilbert space is called a quantum string (qustring, for short) of size n. The notation \(\mathcal{H}_\infty\) is used for the collection of all finite qustrings for brevity.

We use multi-tape quantum Turing machines (QTMs), defined in [1, 23, 32], as a mathematical model of quantum computation. A multi-tape QTM is equipped with two-way infinite tapes, tape heads, and a finite-control unit, similar to a classical TM. A QTM follows its transition function (or algorithm), which dictates the next move of the machine. Formally, a k-tape QTM \(M\) is a six-tuple \((Q, \Sigma_1 \times \Sigma_2 \times \cdots \times \Sigma_k, \Gamma, \Gamma_1 \times \Gamma_2 \times \cdots \times \Gamma_k, q_0, Q_f, \delta)\), where \(Q\) is a finite set of internal states including the initial state \(q_0\) and a set \(Q_f\) of final states, each \(\Sigma_i\) is an input alphabet of tape \(i\), each \(\Gamma_i\) is a tape alphabet of tape \(i\) including a blank symbol and \(\Sigma_i\), and \(\delta\) is a quantum transition function from \(Q \times \Gamma_1 \times \cdots \times \Gamma_k\) to \(\mathbb{C}^{Q \times \Gamma_1 \times \cdots \times \Gamma_k \times (L, N, R)^k}\). An oracle QTM is a QTM equipped with an extra query tape and two distinguished states: a pre-query and post-query states. Let \(A\) be an oracle. When the machine enters a pre-query state, the string written in the query tape, say \(|x)b\rangle\), where \(x \in \Sigma^*\) and \(b \in \{0, 1\}\), is changed into \(|x)b + A(x)\rangle\) in a single step and the machine enters a post-query state. The running time of \(M\) on multi-inputs \(\bar{x}\) is the minimal number \(t\) (if any) such that, at time \(t\), all computation paths of \(M\) on inputs \(\bar{x}\) reach final configurations (i.e., configurations with final states). We say that \(M\) on inputs \(\bar{x}\) halts in time \(t\) if the running time of \(M\) on \(\bar{x}\) is defined and is exactly \(t\).

The transition function is considered as an operator that transforms a superposition of configurations at time \(t\) to another superposition of configurations at time \(t + 1\). We call such an operator a time-evolution operator (or matrix). A QTM has \(K\)-amplitudes if all the entries of its time-evolution matrix are drawn from set \(K\). A QTM is called well-formed if its time-evolution operator is unitary (see Appendix for three local requirements given in [32]). For simplicity, all QTMs dealt in this paper are assumed to be well-formed unless otherwise stated. A k-tape QTM \(M\) is stationary if all tape heads move back to the start cells, and \(M\) is in normal form if, for every \(q \in Q_f\), there exists a series of directions \(\vec{d} \in \{L, N, R\}^k\) such that \(\delta(q, \vec{\sigma}) = \{|q_0\rangle|\vec{\sigma}\rangle|\vec{d}\rangle\) for all tape symbols \(\vec{\sigma} \in \Gamma_1 \times \cdots \times \Gamma_k\). We say that a well-formed QTM \(M\) accepts input \(|\phi\rangle\) with probability \(\alpha\) if \(M\) halts in a final configuration in which, when observed, bit 1 is found in the start cell of the output tape with probability \(\alpha\). In this case, we also say that \(M\) rejects input \(|\phi\rangle\) with probability \(1 - \alpha\).

A function \(f\) from \(\Sigma^*\) to the unit real interval \([0, 1]\) is in \(\#\text{QP}\) (“sharp” QP) if there exists a polynomial-time well-formed QTM \(M\) with \(\mathbb{C}\)-amplitudes such that, for every \(x\), \(f(x)\) is the probability that \(M\) accepts \(x\) [33]. In this case, we simply say that \(M\) witnesses \(f\). A function \(f\) from \(\Sigma^*\) to \([-1, 1]\) is in \(\text{GapQP}\) if there exists a polynomial-time well-formed QTM \(M\) with \(\mathbb{C}\)-amplitudes such that, for every \(x\), \(f(x)\) is the difference between the acceptance probability of \(M\) on input \(x\) and the rejection probability of \(M\) on \(x\) [33]. Let \(\text{FEQP}\) be the collection of all functions from \(\Sigma^*\) to \(\Sigma^*\) whose outputs are produced by polynomial-time, \(\mathbb{C}\)-amplitude, well-formed QTMs with certainty [33, 3]. A set \(A\) is in \(\text{BQP}\) if there exists a function \(f\) in \(\#\text{QP}\) such that, for every \(x\), if \(x \in A\) then \(f(x) \geq 3/4\) and otherwise \(f(x) \leq 1/4\) [4]. A set \(A\) is in \(\text{NQP}\) if there exists a function \(f\) in \(\#\text{QP}\) such that, for every \(x\), \(x \in A\) iff \(f(x) > 0\) [4].

Remark on the convention of quantum extension: Although we normally deal with classical inputs for a QTM \(M\), we sometimes feed \(M\) with quantum states. In this way, however, we can naturally expand the definition of a function \(f\) based on classical strings to a function \(\hat{f}\) based on qustrings without altering \(M\) that defines \(f\). Such \(\hat{f}\) is called the quantum extension of \(f\). By abusing the notation, we use the same symbol \(f\) to cope with both functions. We use the same convention for a set of strings.

Using the aforementioned convention of quantum extension, we define \(\text{QMA}\) as follows: a set \(A\) is in \(\text{QMA}\) if there exist a polynomial \(p\) and a function \(f\) in \(\#\text{QP}\) such that, for every \(x\), if \(x \in A\) then \(f(|x\rangle|\phi\rangle) \geq 3/4\) for a certain qustring \(|\phi\rangle\) of size \(p(|x|)\) and if \(x \notin A\) then \(f(|x\rangle|\phi\rangle) \leq 1/4\) for every
3 Krentel’s Framework for Optimization Problems

Optimization problems have arisen in many areas of computer science. Most \( \text{NP} \)-complete decision problems, for instance, naturally yield their optimization counterparts. In the 1980s, Krentel\cite{Krentel1988} made a systematic approach toward \( \text{NP} \) optimization problems. In particular, he studied the problems of finding the maximal (as well as minimal) outcome of a polynomial-time nondeterministic computation and he introduced the function class, called \( \text{OptP} \), that constitutes all such optimization problems.

**Definition 3.1**\cite{Krentel1988} A function from \( \Sigma^* \) to \( \mathbb{N} \) is in \( \text{OptP} \) if there exists a polynomial-time nondeterministic TM \( M \) such that, for every \( x \), (i) every computation path of \( M \) on input \( x \) terminates with binary strings (which are interpreted as natural numbers) on its output tape and accepts and (ii) \( f(x) \) is the maximum output value of \( M \) on input \( x \).

Using the notion of FP-functions, we rephrase Definition 3.1 in the following way: a function \( f \) is in \( \text{OptP} \) iff there exist a polynomial \( p \) and a function \( g \in \text{FP} \) such that, for every \( x \),

\[
f(x) = \max\{g_s(x) \mid s \text{ is any string of length } p(|x|)\},
\]

where \( g_s(x) \) means \( g((x, s)) \) for each \( s \) viewed as an index. This characterization enables us to generalize \( \text{OptP} \) to \( \text{OptFP} \) by replacing an FP-function \( g \) with another function from a more general function class \( \mathcal{F} \).

**Definition 3.2** Let \( \mathcal{F} \) be any set of functions from \( \Sigma^* \) to \( \mathbb{R} \). A function \( f \) from \( \Sigma^* \) to \( \mathbb{R} \) is in \( \text{OptFP} \) if there exists a polynomial \( p \) and a function \( g \) in \( \mathcal{F} \) such that, for every \( x \), \( f(x) = \max\{g_s(x) \mid s \in \Sigma^{p(|x|)}\} \), where \( g_s(x) = g((x, s)) \). The subscript \( s \) is called a classical index. The class \( \mathcal{F} \) is called the underlying class of \( \text{OptFP} \).

With this general notation, \( \text{OptFP} \) coincides with \( \text{OptP} \). Another example obtained from the above definition is the function class \( \text{OptFP} \) by taking \( \text{FP} \) as an underlying class. Clearly, \( \text{OptP} \cup \text{FP} \subseteq \text{OptFP} \) since \( \text{FP} \subseteq \text{NP} \) (by identifying binary strings with natural numbers). Moreover, we can define the class \( \text{OptQP} \) by taking \( \text{QP} \) as an underlying set. This class naturally expands \( \text{OptFP} \) but stays within \( \text{QP} \).

**Lemma 3.3** 1. For every \( f \in \text{OptQP} \), there exist two functions \( g \in \text{OptQP} \) and \( \ell \in \text{FP} \) such that, for all \( x \), \( f(x) = g(x)\ell(1^{p(|x|)}) \).

2. \( \text{OptQP} \subseteq \text{QP} \).

For the proof, we need the following result from a revision of \cite{Kitaev2002}.

**Lemma 3.4** [\cite{Kitaev2002}, revision] Let \( A \) be any set. The following three statements are all equivalent: (i) \( A \in \text{PP} \); (ii) there exist two functions \( f, g \in \text{QP} \) such that, for every \( x \), \( x \in A \iff f(x) > g(x) \); and (iii) there exist two functions \( f, g \in \text{GapQP} \) such that, for every \( x \), \( x \in A \iff f(x) > g(x) \).

**Proof of Lemma 3.3.** 1) Let \( f \) be any function in \( \text{OptQP} \). That is, there exists a polynomial \( p \) and a function \( h \in \text{QP} \) such that \( f(x) = \max\{h_s(x) \mid s \in \Sigma^{p(|x|)}\} \), where \( h_s(x) = h((x, s)) \). By Kitaev\cite{Kitaev2002} and Watrous\cite{Watrous2003} defined the class QMA based on the quantum circuit model. In this paper, for our convenience, we use the quantum Turing machine model.

Although Krentel also includes the minimization problems into \( \text{OptP} \), this paper focuses only on maximization problems as in \cite{Krentel1988} and Definition 3.1 does not include any minimization problems.
the argument used in [33], we can define \( k \in \#QP \) and \( \ell \in FP \) that satisfy the following condition: 
\[ k((x,s)) = 0 \text{ if } |s| \neq p(|x|), \text{ and otherwise, } k((x,s))\ell(1^{|x|}) = h((x,s)). \]
For the desired \( g \), define 
\[ g(x) = \max\{k_s(x) \mid s \in \Sigma^{|x|}\} \text{ for each } x. \]

2) Let \( f \) be any function in \( \text{Opt}\#QP \) and take a \( g \in \#QP \) and a polynomial \( p \) such that 
\[ f(x) = \max\{g(x) \mid s \in \Sigma^{|x|}\} \text{ for all } x. \]
Choose the lexicographically minimal string \( s_x \) such that 
\[ f(x) = g((x,s_x)) \text{ and } |s_x| = p(|x|). \]
Define 
\[ A = \{(x,s,t,y) \mid \exists z(s \leq z \leq t \land g_z(x) \geq 0,y)\}. \]
Note that \( A \) belongs to \( \text{NP}_{PP} \) by Lemma 3.4. The function \( f \) is computed as follows using \( A \) as an oracle. Let \( x \) be any input of length \( n \). By binary search, we find a string \( y \) such that (i) \( g_{s_x}(x) \geq 0.y \) and (ii) for every \( z \in \Sigma^{|x|} \), \( g_z(x) < g_{s_x}(x) \) implies \( g_z(x) < 0.y \). Then, by decreasing the interval \([s,t]\) in a way similar to the binary search, we can find a string \( s_0 \) of length \( p(|x|) \) such that \( g_{s_0}(x) \geq 0.y \). At last, we compute \( g_{s_0}(x) \) in a quantum fashion. Thus, \( f \) is in \( \#QP^A \subseteq \#QP_{NP^{PP}} \). □

We next show that the collapse \( \text{Opt}\#QP = \#QP \) is unlikely. To state Proposition 3.6, we recall from [33] the class \( \text{WQP} \), which is a quantum analogue of \( \text{WPP} \) in [11].

**Definition 3.5** [33] A set \( S \) is in \( \text{WQP} \) ("wide" \( \text{QP} \)) if there exist two functions \( f \in \#QP \) and \( g \in \text{EFF} \) such that, for every \( x \), (i) \( g(x) \in (0,1] \cap \mathbb{Q} \) and (ii) if \( x \in S \) then \( f(x) = g(x) \) and otherwise \( f(x) = 0 \), where we identify a string with a rational number expressed as a pair of integers (e.g., \( g(x) = \frac{1}{3} \)).

Note that \( \text{EQP} \subseteq \text{WQP} \subseteq \text{NQP} \subseteq \text{PP} \). However, we do not know any relationship between \( \text{WQP} \) and \( \text{BQP} \).

**Proposition 3.6** \( \text{PP} = \text{EQP} \Rightarrow \#QP = \text{Opt}\#QP \Rightarrow \text{PP} = \text{WQP} \).

**Proof.** If \( \text{EQP} = \text{PP} \) then \( \text{NP}_{PP} \subseteq \text{PP}_{NP} \subseteq \text{EQP} = \text{EQP} \). Since \( \#QP^{EQP} = \#QP \) [33], by Lemma 3.3 we obtain \( \text{Opt}\#QP \subseteq \#QP \).

For the second implication, assume that \( \#QP = \text{Opt}\#QP \). Let \( A \) be an arbitrary set in \( \text{PP} \). As shown in [33], \( \text{PP} \) coincides with its quantum analogue \( \text{PP}_{Q} \). Thus, there exists a function \( f \in \#QP \) such that, for every \( x \), (i) if \( x \in A \) then \( f(x) > 1/2 \) and (ii) if \( x \notin A \) then \( f(x) < 1/2 \). Define \( g(x) = \max\{f(x),\frac{1}{2}\} \) for every \( x \). This \( g \) is clearly in \( \text{Opt}\#QP \) and thus in \( \#QP \). By the definition of \( g \), if \( x \in A \) then \( g(x) > 1/2 \) and otherwise \( g(x) = 1/2 \). Next, define \( h(x) = g(x) - \frac{1}{2} \) for all \( x \). Since \( \text{GapQP} = \#QP - \#QP \) [33], \( h \) is in \( \text{GapQP} \). Thus, \( h^2 \) is in \( \#QP \) [33]. For this \( h^2 \), it follows that \( x \in A \) implies \( h^2(x) > 0 \) and \( x \notin A \) implies \( h^2(x) = 0 \). At this moment, we obtain that \( A \in \text{NQP} \).

Since \( h^2 \) is in \( \#QP \), there exists a polynomial \( p \) such that, for every \( x \), if \( h^2(x) > 0 \) then \( h^2(x) > 2^{-p(|x|)} \) because the acceptance probability of a QTM is expressed in terms of a polynomial in the transition amplitudes from \( \mathbb{C} \). To complete the proof, we define \( k(x) = \min\{h^2(x),2^{-p(|x|)}\} \) for every \( x \). It follows that \( x \in A \) implies \( k(x) = 2^{-p(|x|)} \) and \( x \notin A \) implies \( k(x) = 0 \). To see that \( k \) is in \( \#QP \), consider the fact that \( 1 - k(x) = \max\{1 - h^2(x),1 - 2^{-p(|x|)}\} \) is in \( \text{Opt}\#QP \), which is \( \#QP \) by our assumption. Thus, \( 1 - (1 - k(x)) \) is also in \( \#QP \), which implies that \( k \) is in \( \#QP \). □

At the end of this section, we note that Krentel’s framework has been extended in several different manners in the literature [3, 7].

### 4 Quantum Optimization Problems

Krentel’s optimization problems are to maximize the value of indexed functions chosen from underlying class \( F \). As shown in the previous section, Krentel’s framework can cope with the class \( \text{Opt}\#QP \). However, \( \text{Opt}\#QP \) is a concoction of a classical indexing system and quantum computations. In this section, we truly expand Krentel’s framework and introduce quantum optimization problems. Our
quantum optimization problem uses a quantum computation together with a quantum index, which is a qustring of polynomial size. We begin with the general definition, paving a road to our study of $\text{Qopt}\#\text{QP}$.

**Definition 4.1** Let $\mathcal{F}$ be a set of functions from $\Sigma^* \times \mathcal{H}_\infty$ to $\mathbb{R}$. A quantum optimization problem $f$ from $\Sigma^*$ to $\mathbb{R}$ is in $\text{Qopt}\mathcal{F}$ if there exist a polynomial $p$ and a function $g \in \mathcal{F}$ such that, for all $x$,

$$f(x) = \sup\{g(\phi)(x) \mid |\phi\rangle \text{ is any qustring of size } p(|x|)\},$$

where $g(\phi)(x) = g(x, |\phi\rangle)$. The subscript $|\phi\rangle$ is called a quantum index. For simplicity, we say that $g$ witnesses $f$.

In the course of a study on a quantum optimization problem, it is rather convenient to optimize the acceptance probability of a polynomial-time well-formed QTM indexed with a quantum state. From this reason, we mainly study the class $\text{Qopt}\#\text{QP}$ throughout this paper and leave other platforms to the interested reader. This class $\text{Qopt}\#\text{QP}$ consists of all quantum optimization problems $f$ such that there exist a polynomial $p$ and a multi-tape, polynomial-time, well-formed QTM $M$ with $\mathbb{C}$-amplitudes satisfying that, for all $x$, $f(x)$ is equal to the supremum, over all qustrings $|\phi\rangle$ of size $p(|x|)$, of the probability that $M$ accepts $(|x|, |\phi\rangle)$. The class $\text{Qopt}\#\text{QP}$ naturally includes $\text{Opt}\#\text{QP}$.

**Observation:** The size factor $p$ of a quantum index $|\phi\rangle$ in Definition 4.1 can be replaced by any polynomial $q$ that majorizes $p$. This is shown easily by ignoring the extra $q(|x|) - p(|x|)$ qubits on input $x$ because those qubits that are not accessed by a QTM do not affect the acceptance probability of the QTM.

Solving a quantum optimization problem is closely related to finding the maximal eigenvalue of a certain type of positive semidefinite, contractive, Hermitian matrix. In what follows, we clarify this relationship. Assume that we have a multi-tape well-formed QTM witnessing a quantum optimization problem $f$. Let $p$ be a polynomial expressing the size of a quantum index. Without loss of generality, we can assume that $M$ is stationary in normal form [4, 32]. As shown in [32], there exists a reversing QTM for $M$, denoted $M^\dagger$. We then introduce the new QTM, called $N_{M,p}$, that behaves as follows:

On input $(x, t)$ given in the input tape, if $|t| \neq p(|x|)$ then skip the following procedure and halt. Let $n = |x|$ and assume that $t \in \Sigma^p(n)$. Copy $x$ onto a new tape, called the storage tape. Run $M$ on input $(x, t)$. When it halts in polynomial time, copy $M$’s output bit (either $|0\rangle$ or $|1\rangle$) onto another new tape, called the result tape. Run the reversing machine $M^\dagger$ on the final configuration excluding the storage tape and the result tape. After $M^\dagger$ halts in polynomial time, if $N_{M,p}$’s configuration consists only of $(x, s)$ in the input tape, where $s$ is a certain string of length $p(|x|)$, of $x$ in the storage tape, of $1$ in the result tape (and empty elsewhere), then move $(x, s)$ into the output tape and empty all the other tapes and halt. Otherwise, write the blank symbol in the output tape and halt.

By an appropriate implementation, we can make all the computation paths of $N_{M,p}$ on each input terminate simultaneously. Now, fix $x$ and let $n = |x|$. For each pair $(s, t) \in \Sigma^p(n) \times \Sigma^p(n)$, define $\alpha_{x,s,t}$ to be the amplitude of a unique final configuration in which, starting with input $(x, t)$, $N_{M,p}$ outputs $(x, s)$ in a unique final inner state. Let $P_{M,p,x}$ be the $2^p(n) \times 2^p(n)$ matrix $(\alpha_{x,s,t})_{s,t \in \Sigma^p(n)}$. It is not difficult to show by the definition of $N_{M,p}$ that $P_{M,p,x}$ is Hermitian, positive semidefinite, and contractive. Thus, each $\alpha_{x,s,t}$ is a real number and $\alpha_{x,s,t} = \alpha_{x,t,s}$ for all pairs $(s, t) \in \Sigma^p(n) \times \Sigma^p(n)$. Note that the acceptance probability of $M$ on input $(x, |\phi\rangle)$ is exactly $|\langle \phi | P_{M,p,x} | \phi \rangle|$. Thus,

$$f(x) = \sup\{||\langle \phi | P_{M,p,x} | \phi \rangle|| \mid |\phi\rangle \text{ is any qustring of size } p(n)\}$$

$$= ||P_{M,p,x}||,$$
which coincides with the maximal eigenvalue \( \lambda \) of \( P_{M,p,x} \) (see, e.g., [5]). A similar construction has been shown in the literature [3, 12].

In a quantum setting, “squaring” becomes a unique operation because of the reversibility nature of quantum computation. For example, as shown in [33], \( f \in \text{GapQP} \) implies \( f^2 \in \#\text{QP} \). In the next lemma, we show that squaring does not increase the size of a quantum index.

**Lemma 4.2** Let \( p \) be any polynomial, \( g \) any function in \( \#\text{QP} \), and \( f \) any function in \( \text{Qopt} \#\text{QP} \). Assume that \( f(x) = \sup \{ g(x,|\phi\rangle) \mid |\phi\rangle \text{ is any qustring of size } p(|x|) \} \) for all \( x \). Then, there exists a function \( h \) in \( \#\text{QP} \) such that \( f^2(x) = \sup \{ h(x,|\phi\rangle) \mid |\phi\rangle \text{ is any qustring of size } p(|x|) \} \) for all \( x \).

**Proof.** Since \( g \in \#\text{QP} \), let \( M \) be a multi-tape, \( \tilde{C} \)-amplitude, stationary, well-formed QTM \( M \) in normal form that witnesses \( g \). By the aforementioned argument, \( f(x) = \| P_{M,p,x} \| \). Since \( P_{M,p} \) is Hermitian, \( f^2(x) = \| P_{M,p,x} \|^2 = \| P_{M,p}^2 \| \). We slightly modify the QTM \( N_{M,p} \) and define the new QTM, called \( N \), in the following fashion:

- **On input** \((x,t)\), if \(|t| \neq p(|x|)\) then reject the input. Let \( n = |x|\) and assume that \( t \in \Sigma^{p(n)} \).
- **Run** \( N_{M,p} \) on input \((x,t)\). If \( N_{M,p} \) outputs \((x,s)\) for a certain string \( s \) of length \( p(|x|) \), then accept the input. Otherwise, reject the input.

For the desired \( h \), define \( h(x,t) \) to be the acceptance probability of \( N \) on input \((x,t)\). Note that \( N_{M,p} \) accepts input \((x,|\phi\rangle)\) with probability exactly \( |\langle \phi|P^1_{M,p,x}P_{M,p,x}|\phi\rangle| \), which equals \( |\langle \phi|P^2_{M,p,x}|\phi\rangle| \).

Hence,

\[
\| P_{M,p,x}^2 \| = \sup \{ |\langle \phi|P^2_{M,p,x}|\phi\rangle| \mid |\phi\rangle \text{ is any qustring of size } p(|x|) \}
\]

\[
= \sup \{ h(x,|\phi\rangle) \mid |\phi\rangle \text{ is any qustring of size } p(|x|) \}.
\]

Since \( f^2(x) = \| P_{M,p,x}^2 \| \), we obtain the desired equation. \( \square \)

## 5 Fundamental Properties of Qopt\#QP

We examine the fundamental properties of quantum optimization problems in \( \text{Qopt} \#\text{QP} \). In what follows, we show that \( \text{Qopt} \#\text{QP} \) enjoys important closure properties, such as multiplication, exponentiation, limited addition, and limited composition.

Firstly, we show that \( \text{Qopt} \#\text{QP} \) is closed under composition with \( \text{FP} \)-functions. To be more precise, for any two function classes \( \mathcal{F} \) and \( \mathcal{G} \), let \( \mathcal{F} \circ \mathcal{G} \) denote the class of functions \( f \circ g \), where \( f \in \mathcal{F} \) and \( g \in \mathcal{G} \) and \( f \circ g \) is the composition defined as \( f \circ g(x) = f(g(x)) \) for all \( x \) in the domain of \( g \). Using this notation, our claim is expressed as follows. The proof of the claim is immediate.

**Lemma 5.1** \( \text{Qopt} \#\text{QP} \circ \text{FP} = \text{Qopt} \#\text{QP} \).

In the previous section, we have shown that solving a quantum optimization problem is equivalent to finding the maximal eigenvalue of a certain positive semidefinite, contract, Hermitian matrix. We use this characterization to show the fundamental properties of quantum optimization problems. To describe the claim, we need the notion of an \( \ell \)-qubit source.

A **qubit ensemble** is a sequence of qustrings with index set \( I \). A qubit ensemble \( \{ |\phi_x\rangle \}_{x \in I} \) is called an \( \ell \)-**qubit source** if each \( |\phi_x\rangle \) is a qustring of size \( \ell(|x|) \) and there exists a polynomial-time, \( \tilde{C} \)-amplitude, well-formed, clean QTM that generates \( |\phi_x\rangle \) on input \( x \), where a QTM is called **clean** if it is stationary in normal form and all the tapes except the output tape are empty when it halts with one distinguished final state.
Lemma 5.2  Let \( q \) be a polynomial. Let \( \ell \) be any function in \( \mathbb{N} \) such that \( \ell(n) \in O(\log n) \) and let 
\[ \{ \phi_x \}_{x \in \Sigma^*} \] 
be any \( \ell \)-qubit source. Assume that \( f \) is a function in \( \text{Qopt} \# \text{QP} \). The following functions all belong to \( \text{Qopt} \# \text{QP} \).

1. \( g(x) = \max \{ f(\langle x, y \rangle) \mid y \in \Sigma^{\ell(|x|)} \} \).
2. \( g(x) = \sum_{y:|y| = \ell(|x|)} |\langle y|\phi_x \rangle|^2 \cdot f(\langle x, y \rangle) \).
3. \( g(x) = \prod_{y:|y| = \ell(|x|)} f(\langle x, y \rangle) \).
4. \( g(x, y) = f(x)|y| \).

Proof. 1) Take a polynomial \( p \) and a function \( h \in \# \text{QP} \) such that \( f(\langle x, y \rangle) = \sup \{ h(x, y, |\phi \rangle) \mid |\phi \rangle \text{ is any qustring of size } p(|x|) \} \) for any strings \( x \) and \( y \in \Sigma^{\ell(|x|)} \). Since \( h \in \# \text{QP} \), there exists an appropriate QTM \( M \) that witnesses \( h \). For simplicity, assume that there exists a polynomial \( r \) such that \( |\langle x, y \rangle| = r(|x|) \) for all \( y \in \Sigma^{\ell(|x|)} \).

Define the new QTM \( N \) as follows. Let \( (x, |\psi \rangle) \) be any quantum input, where \( n = |x| \) and \( |\psi \rangle \) is any qustring of size \( q(n) + p(n) \). Note that \( |\psi \rangle \) is written in the form \( \sum_{y:|y| = q(n)} \beta_y |y \rangle \otimes |\phi_y \rangle \) for a certain series of qustrings \( \{ |\phi_y \rangle \}_{y \in \Sigma^q(n)} \) and a certain series of complex numbers \( \{ \beta_y \}_{y \in \Sigma^q(n)} \) satisfying \( \sum_{y:|y| = q(n)} |\beta_y|^2 = 1 \).

First, observe the first \( q(n) \) qubits (i.e., \( |y \rangle \)) of the tape content \( |\psi \rangle \) and copy the result onto a new tape to remember it. After the observation, we obtain \( y \) and a quantum state \( \beta_y |\phi_y \rangle \).

Then, simulate \( M \) on inputs \( (x, y) \) and \( \beta_y |\phi_y \rangle \).

Let \( k(x, |\psi \rangle) \) denote the acceptance probability of \( N \) on input \( (x, |\psi \rangle) \). Obviously, \( k(x, |\psi \rangle) = \sum_{y:|y| = q(n)} |\beta_y|^2 h(x, y, |\phi_y \rangle) \).

Consider the supremum \( \sup \{ k(x, |\psi \rangle) \} \), where \( |\psi \rangle \) runs over all qustrings of size \( q(n) + p(n) \).

By a simple calculation, \( \sup \{ k(x, |\psi \rangle) \} = \sup \{ \beta_y \} \sup \{ \sum_{y:|y| = q(n)} |\beta_y|^2 h(x, y, |\phi_y \rangle) \} \), which is equal to \( \sup \{ \beta_y \} \sup \{ \sum_{y:|y| = q(n)} |\beta_y|^2 f(\langle x, y \rangle) \} \), where \( \{ \beta_y \}_{y \in \Sigma^q(n)} \) runs over all sequences of complex numbers with \( \sum_{y:|y| = q(n)} |\beta_y|^2 = 1 \) and each \( |\phi_y \rangle \) runs all qustrings of size \( q(n) \). By the property of convex combination with \( \sum_{y:|y| = q(n)} |\beta_y|^2 = 1 \), the value \( \sup \{ \beta_y \} \sup \{ \sum_{y:|y| = q(n)} |\beta_y|^2 f(\langle x, y \rangle) \} \) equals \( \max \{ f(\langle x, y \rangle) \mid y \in \Sigma^q(n) \} \). Therefore, \( N \) witnesses \( g \).

2) For simplicity, we assume the existence of a polynomial \( r \) such that \( 2^{\ell(n)} \leq r(n) \) for all \( n \in \mathbb{N} \). Without loss of generality, we can assume that there exist a polynomial \( p \) and a function \( h \in \# \text{QP} \) which, for any strings \( x \) and \( y \in \Sigma^{\ell(|x|)} \), force \( \sup \{ h(x, y, |\phi \rangle) \mid |\phi \rangle \text{ is any qustring of size } p(|x|) \} \) to be \( f(\langle x, y \rangle) \). Let \( M \) be an appropriate QTM \( M \) that witnesses \( h \).

Consider the following QTM \( N \). Let \( x \) (say, \( n = |x| \)) be any input string and \( |\psi \rangle \) any input qustring of size \( r(n)p(n) \). We section \( |\psi \rangle \) into \( r(n) \) blocks of equal size \( p(n) \). The first \( 2^{\ell(n)} \) blocks are assumed to be indexed with strings of length \( \ell(n) \).

Generate qustring \( |\phi_x \rangle \) in a new tape and then observe the tape content. Let \( y \) be the result after the observation. Now, copy \( y \) onto a new tape and then simulate \( M \) on input \( (x, y) \) as well as the content of the \( y \)th block of \( |\psi \rangle \).

For each \( y \), let \( |\psi_y \rangle \) be any qustring of size \( p(n) \) that achieves the maximal acceptance probability of \( M \) on input \((x, y, |\psi_y \rangle)\); that is \( f(\langle x, y \rangle) = h(x, y, |\psi_y \rangle) \). Note that, for any qustring \( |\psi \rangle \) of size at least \( p(n) \), the acceptance probability of \( M \) on input \((x, y)\) accessing only the first \( p(n) \) qubits of \( |\psi \rangle \) cannot be more than \( f(\langle x, y \rangle) \). Hence, to maximize the acceptance probability of \( N \), \( |\psi \rangle \) must be the tensor product \( (\bigotimes_{y:|y| = \ell(n)} |\psi_y \rangle) \otimes |\xi \rangle \), where \( |\xi \rangle \) is any qustring of size \( (r(n) - 2^{\ell(n)})p(n) \). In this case, the acceptance probability of \( N \) on input \((x, |\psi \rangle)\), after \( y \) is observed, is \( |\langle y|\phi_x \rangle|^2 h(x, y, |\psi_y \rangle) \). Note that any two simulations on different \( y \)'s do not interfere each other. Hence, \( N \) witnesses \( g \).
We then show that $Q_{\text{opt}}$ runs contribute to a multiplicative factor of $f$ exactly $f$.

From the proof of Lemma 4.2, we can achieve the maximal acceptance probability of $N$ on input $(x,|\psi\rangle)$. Thus, $N$ witnesses $g$.

4) This is basically an extension of the proof of Lemma 4.2. Since $f \in Q_{\text{opt}}\#Q$, let $p$ be a polynomial and $M$ be a QTM that witnesses $f$. Let $N_{M,p}$ be the QTM induced from $M$ as described in Section 9. For our proof, we slightly modify $N_{M,p}$ in such way that, instead of moving $(x,s)$ from the input tape to the output tape, it keeps $(x,s)$ in the input tape and erases only the storage-tape content (keeping 1 in the result tape).

Now, consider the following QTM $P$. Let $x$ be any input string of length $n$ and $y$ be any string of length $m$. Let $m = 2k + j$, where $k \in \mathbb{N}$ and $j \in \{0,1\}$. We prepare a new tape, called the checking tape.

On input $(x,y,|\psi\rangle)$ given in tape 1, repeat the following procedure (*) by incrementing $i$ by one from 1 to $k$. For convenience, we call the initial configuration round 0.

(*) At round $i$, $P$ simulates $N_{M,p}$ starting with the configuration left from the previous round, and when it halts, move the one-bit content of the result tape into the $i$th cell of the checking tape.

After this procedure, when $j = 1$, we make one additional round: simulate $M$ starting with the configuration left from the previous round and, when it halts, write the outcome (either 0 or 1) into the $k+j$th cell of the checking tape. Finally, observe the checking tape and accept the input iff the $k+j$ cells consists only of 1s.

Let $|\psi_x\rangle$ be any quantum index that maximizes the acceptance probability of $M$ on input $(x,|\psi_x\rangle)$. From the proof of Lemma 4.2, $N_{M,p}$ accepts $(x,|\psi_x\rangle)$ with probability $f^2(x)$. More generally, we can show by induction that, after each round $i$, if we observe the checking tape with observable $|1^i\rangle$ then we obtain the quantum state $f^{2k}(x)|x\rangle|\psi_x\rangle$ in the input tape. In case where $j = 1$, the additional round contributes to a multiplicative factor of $f(x)$. Therefore, $P$ accepts $(x,|\psi_x\rangle)$ with probability exactly $f^{2k+j}(x)$, which is $f^m(x)$.

It is also important to note that the size of quantum index is independent of $y$. 

The class $Q_{\text{opt}}\#Q$ is shown to be robust in the following sense.

**Proposition 5.3**  $Q_{\text{opt}}(\text{Opt}\#Q) = \text{Opt}(Q_{\text{opt}}\#Q) = Q_{\text{opt}}\#Q$.

As for the definition of $Q_{\text{opt}}(\text{Opt}\#Q)$, it is important to note that, by our convention of quantum extension, $f$ is in $Q_{\text{opt}}(\text{Opt}\#Q)$ iff there exists a function $h \in \#Q$ such that, for every $x$, $f(x) = \sup_{|\phi\rangle} \max_s \{h(x,|\phi\rangle,s)\}$, where $|\phi\rangle$ runs over all qustrings of polynomial size and $s$ runs over all strings of polynomial length.

**Proof of Proposition 5.3.** It follows from $\#Q \subseteq \text{Opt}\#Q$ that $Q_{\text{opt}}\#Q \subseteq Q_{\text{opt}}(\text{Opt}\#Q)$. We then show that $Q_{\text{opt}}(\text{Opt}\#Q) \subseteq \text{Opt}(Q_{\text{opt}}\#Q)$. This follows from the fact that we can
swap the “max” operator and the “sup” operator. The inclusion $\text{Opt}(Qopt\#QP) \subseteq Qopt\#QP$ follows from Lemma 5.2(1).

Proposition 5.3 seems unlikely to be extended to $\text{opt}(Qopt\#QP) = Qopt\#QP$ because of the inability to distinguish a tensor product of two short quantum indices from one large quantum index. We conjecture that $\text{opt}(Qopt\#QP) \neq Qopt\#QP$.

This also suggests a generalization of $Qopt\#QP$ into $Qopt_k\#QP$ for each $k \in \mathbb{N}^+$ by taking a tensor product of $k$ quantum indices: a function $f$ is in $Qopt_k\#QP$ if there exists a polynomial $p$ and a function $g \in \#QP$ such that, for every $x$, $f(x) = \sup\{g(x, |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_k\rangle)\}$, where the supremum is over all $k$-tuples $(|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_k\rangle)$ of strings of size $p(|x|)$. With this notation, we can show that $\text{opt}(Qopt\#QP) = Qopt_2\#QP$.

6  Approximate Reduction and Universality

Based upon his metric reducibility between NP optimization problems, Krentel [20] introduced the notion of complete problems for OptP. There are also many other reductions used for NP optimization problems in the literature. Krentel’s complete problems constitute the hardest problems in OptP. It is natural to consider a similar notion among quantum optimization problems. However, problems in $Qopt\#QP$ are functions computed by well-formed $\hat{\mathcal{C}}$-amplitude QTMs and thus, there is no single QTM that exactly simulates all the other well-formed QTMs with $\hat{\mathcal{C}}$-amplitudes. Instead, we relax the meaning of “completeness”.

Following Deutsch’s work [3], Bernstein and Vazirani [4] constructed a universal QTM that can approximately simulate any well-formed QTM $M$ for $t$ steps with desired accuracy $\epsilon$ at the cost of polynomial slowdown. In other words, every QTM can be “approximately” reduced to one single QTM. We can generalize this notion of universality in the following fashion.

**Definition 6.1** 1) Let $f$ and $g$ be any functions from $\{0, 1\}^*$ to $[0, 1]$. The function $f$ is (polynomial-time) approximately reducible to $g$, denoted $f \preceq^p g$, if there is a function $k \in \mathbb{F}P$ such that, for every $x$ and $m \in \mathbb{N}^+$, $|f(x) - g(k(x01^m))| \leq 1/m$.

2) Let $\mathcal{F}$ be any class of functions from $\{0, 1\}^*$ to $[0, 1]$. A function $g$ from $\Sigma^*$ to $[0, 1]$ is universal for $\mathcal{F}$ (or $\mathcal{F}$-universal, in short) if (i) $g$ is in $\mathcal{F}$ and (ii) every function $f \in \mathcal{F}$ is approximately reducible to $g$.

Unfortunately, we may not replace the term $1/m$ in the above definition by $2^{-m}$. This relation $\preceq^p$ is reflexive and transitive. The proof is immediate from the definition.

**Lemma 6.2** The relation $\preceq^p$ satisfies that (i) for any $f$, $f \preceq^p f$ and (ii) for any $f$, $g$, and $h$, if $f \preceq^p g$ and $g \preceq^p h$, then $f \preceq^p h$.

The importance of a universal function is given as in Lemma 5.3. Before describing the lemma, we introduce useful notations for “approximate membership” and “approximate inclusion.”

**Definition 6.3** Let $\mathcal{F}$ and $\mathcal{G}$ be any two classes of functions from $\Sigma^*$ to the unit real interval $[0, 1]$ and let $f$ be any function from $\Sigma^*$ to $[0, 1]$. The notation $f \overset{\preceq}{\in}^p \mathcal{F}$ means that, for every polynomial $p$, there exists a function $g$ in $\mathcal{F}$ satisfying $|f(x) - g(x)| \leq 1/p(|x|)$ for all $x$. The notation $\mathcal{F} \overset{\preceq}{\in}^p \mathcal{G}$ means that $f \overset{\preceq}{\in}^p \mathcal{G}$ for any function $f$ in $\mathcal{F}$.

**Lemma 6.4** Let $\mathcal{F}$ and $\mathcal{G}$ be any two classes of functions from $\Sigma^*$ to $[0, 1]$. Assume that $\mathcal{G} \circ \mathbb{F}P \subseteq \mathcal{G}$ and let $f$ be any $\mathcal{F}$-universal function. Then, $\mathcal{F} \overset{\preceq}{\in}^p \mathcal{G}$ iff $f \overset{\preceq}{\in}^p \mathcal{G}$.
Proof. (Only If - part) This is trivial since \( f \in \mathcal{F} \). (If -part) Assume that \( f \preccurlyeq^p g \). Take any function \( g \) in \( \mathcal{F} \) and any polynomial \( p \). Since \( f \) is \( \mathcal{F} \)-universal, \( g \preccurlyeq^p f \). There exists a function \( k \in \text{FP} \) such that \( |g(x) - f(k(x01^2p(x)|))| \leq 1/2p(x) \) for all \( x \). Moreover, since \( f \preccurlyeq^p g \), there exists a function \( r \in \mathcal{G} \) such that \( |f(k(x01^2p(x)|)) - r(k(x01^2p(x)|))| \leq 1/2p(x) \). Define \( f'(x) = f(k(x01^2p(x)|)) \) and \( r'(x) = r(k(x01^2p(x)|)) \). Clearly, \( r' \) is in \( \mathcal{G} \cap \text{FP} \subseteq \mathcal{G} \). Thus, \( g \preccurlyeq^p g \) since \( |g(x) - r'(x)| \leq |g(x) - f'(x)| + |f'(x) - r'(x)| \leq 1/p(x) \). This implies that \( \mathcal{F} \preccurlyeq^p \mathcal{G} \).

Most natural classes satisfy the premise of Lemma 6.4. For example, \#QP, GapQP, Opt\#QP, and Qopt\#QP satisfy the premise.

Most well-known quantum complexity classes are believed to lack complete problems. The notion of universality naturally provides promise complete problems for, e.g., BQP by posing appropriate restrictions on the acceptance probabilities of quantum functions in \#QP.

The notion of a universal QTM given by Bernstein and Vazirani \[4\] gives rise to the \#QP-universal function QAP. We assume each DTM has its code (or its description) expressed in binary. A code of an amplitude \( \alpha \) in \( \tilde{C} \) is a code of a DTM that approximates \( \alpha \) to within \( 2^{-n} \) in time polynomial in \( n \). A code of a QTM means the description of the machine with codes of all amplitudes used for the QTM. We assume that any code is expressed in binary.

We fix the universal QTM \( M_U \) that, on input \( \langle M, x, 1^t, 1^m \rangle \), simulates \( M \) on input \( x \) for \( t \) steps and halts in a final configuration \( |\phi_{M_U}\rangle \) satisfying that \( |||\phi_{M_U}\rangle - |\phi_M\rangle|| \leq 1/m \), where \( |\phi_M\rangle \) is the configuration of \( M \) on \( x \) after \( t \) steps \[3\]. For completeness, we assume that if \( M \) is not a well-formed QTM then \( M_U \) rejects the input with probability 1. From the construction of a universal QTM in \[3\], we can assume that \( M_U \) has \( \{0, \pm 1, \pm \cos \theta, \pm \cos \theta, \pm e^{i\theta}\} \)-amplitudes, where \( \theta = 2\pi \sum_{i=1}^{\infty} 2^{-2^i} \).

Adleman et al. \[1\] further simplified the above set of amplitudes; for example, we can replace \( \cos \theta \) and \( \sin \theta \) by 3/5 and 4/5, respectively.

We then define the QTM APPROXIMATION PROBLEM (QAP) as follows:

QTM APPROXIMATION PROBLEM: QAP

- input: \( \langle M, x, 1^t, 1^m \rangle \), where \( M \) is a \( \tilde{C} \)-amplitudes well-formed QTM, \( t \in \mathbb{N} \), and \( m \in \mathbb{N}^+ \).
- output: the acceptance probability of \( M_U \) on input \( \langle M, x, 1^t, 1^m \rangle \).

As Bernstein and Vazirani \[4\] demonstrated, every function \( f \) outputting the acceptance probability of a certain polynomial-time well-formed QTM with \( \tilde{C} \)-amplitudes is approximately reducible to QAP. It is easy to see that QAP is in \#QP. We have the following proposition.

**Proposition 6.5** QAP is \#QP-universal.

The proof of Proposition 6.5 uses the following folklore lemma. Although the proof of the lemma is easy, it is given in Appendix for completeness.

**Lemma 6.6** Let \( M \) and \( N \) be two well-formed QTMs. Let \( U_M \) and \( U_N \) be the superpositions of final configurations of \( M \) on input \( |\phi\rangle \) and of \( N \) on input \( |\psi\rangle \), respectively. Let \( \eta_M(|\phi\rangle) \) and \( \eta_N(|\psi\rangle) \) be the acceptance probabilities of \( M \) on input \( |\phi\rangle \) and of \( N \) on input \( |\psi\rangle \), respectively. Then, \( |\eta_M(|\phi\rangle) - \eta_N(|\psi\rangle)| \leq ||U_M|\phi\rangle - U_N|\psi\rangle|| \).

Now, we give the proof of Proposition 6.5.

**Proof of Proposition 6.5.** Let \( p \) be any polynomial and let \( g \) be any function in \#QP. Let \( M \) be a polynomial-time \( \tilde{C} \)-amplitude well-formed QTM that witnesses \( g \) with quantum index size \( p \). Let \( q \) be a polynomial that bounds the running time of \( M \). We show that \( g \preccurlyeq^p \text{QAP} \).

Fix \( x \) and \( m \) arbitrarily. Let \( |\phi_{M_U}\rangle \) be the final configuration of \( M_U \) on input \( \langle M, x, 1^q(|x|), 1^m \rangle \) and define \( |\phi_M\rangle \) to be the final configuration of \( M \) on input \( x \). We set \( k(x01^m) = \langle M, x, 1^q(|x|), 1^m \rangle \).

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It follows from the definition of \( M_U \) that \( \|\phi_{M_U}\| - \|\phi_M\| \leq 1/m \). Thus, Lemma 6.6 implies that
\[
|\text{QAP}(\langle M, x, 1^t, 1^m \rangle) - g(x)| \leq \|\phi_{M_U}\| - \|\phi_M\| \leq 1/m.
\]
Therefore, we obtain
\[
|\text{QAP}(k(x01^m)) - g(x)| = |\text{QAP}(\langle M, x, 1^t, 1^m \rangle) - g(x)| \leq \frac{1}{m}.
\]
This guarantees \( g \preceq^p \text{QAP} \). \( \square \)

We exhibit a canonical universal problem for \( \text{Qopt} \# \text{QP} \). To avoid any notational inconvenience, we write \( \text{QAP}(\langle M, x, 1^t, 1^m \rangle, s) \) when \( M \) takes an input \( \langle x, s \rangle \). Based on this convention, we define the maximum quantum turing machine problem (MAXQTM) as follows.

**Max Quantum Tm Problem (MAXQTM):**
- **Input:** \( \langle M, x, 1^t, 1^m \rangle \), where \( M \) is a \( \mathbb{C} \)-amplitude well-formed QTM, \( t \in \mathbb{N} \), and \( m \in \mathbb{N}^+ \).
- **Output:** the maximal acceptance probability, over all quantum indices \( |\phi\rangle \) of size \( |x| \), of \( M_U \) on input \( \langle (M, x, 1^t, 1^m), |\phi\rangle \) for every \( |x| \).

Obviously, MAXQTM belongs to \( \text{Qopt} \# \text{QP} \). We further claim that MAXQTM is indeed universal for \( \text{Qopt} \# \text{QP} \).

**Theorem 6.7** MAXQTM is \( \text{Qopt} \# \text{QP} \)-universal.

**Proof.** To see this, let \( f \) be any function in \( \text{Qopt} \# \text{QP} \). There exist a polynomial \( p \) and a function \( g \in \# \text{QP} \) such that \( f(x) = \sup\{g(x, |\phi\rangle) \mid |\phi\rangle \text{ is any qustring of size } p(|x|) \} \) for every \( x \). Without loss of generality, assume that \( p(n) > n + 1 \) for all \( n \). Take an appropriate QTM \( M_g \) that witnesses \( g \).

We show that \( f \preceq^p \text{MAXQTM} \). Define another QTM \( M_g' \) as follows: on input \( z \) and \( s \in \Sigma^{\#z} \), if \( z \) is not of the form \( x01p(|x|) - |x| - 1 \), then reject the input. Otherwise, simulate \( M_g \) on input \( \langle x, s \rangle \).

Let \( q \) be any polynomial such that, for every \( x, M'_g \) on input \( x01p(|x|) - |x| - 1 \) halts in at most \( q(|x|) \) steps. Thus, Proposition 6.5 implies that, for every \( s \in \Sigma^p(|x|) \),
\[
|\text{QAP}(\langle M'_g, x01p(|x|) - |x| - 1, 1^q(|x|), 1^m \rangle, s) - g(x, s)| \leq \frac{1}{m}.
\]
This clearly yields the following inequality:
\[
|\sup_{|\phi\rangle} \{\text{QAP}(\langle M'_g, x01p(|x|) - |x| - 1, 1^q(|x|), 1^m, |\phi\rangle \}) - \sup_{|\phi\rangle} \{g(x, |\phi\rangle)\}| \leq \frac{1}{m},
\]
where \( |\phi\rangle \) runs over all qustrings of size \( p(|x|) \). To complete the proof, it suffices to define \( k(x01^m) = \langle M'_g, x01p(|x|) - |x| - 1, 1^q(|x|), 1^m \rangle \) for all \( x \) and \( m \). \( \square \)

**Corollary 6.8** MAXQTM \( \preceq^p \text{QP} \) iff \( \text{Qopt} \# \text{QP} \in \text{QP} \).

We have just shown an example of universal optimization problem, MAXQTM, for \( \text{Qopt} \# \text{QP} \). Nonetheless, MAXQTM heavily relies on a universal QTM and it seems artificial. To develop a fruitful theory of quantum optimization problems, we need “natural” examples of universal problems in a variety of fields, such as graph theory, logic, and group theory. Finding such natural problems is one of the most pressing open problems in our theory.

## 7 Relationship between \( \text{Qopt} \# \text{QP} \) and \( \# \text{QP} \)

The quantum optimization problems \( \text{Qopt} \# \text{QP} \) are induced from \( \# \text{QP} \)-functions by taking quantum indices. However, there has been shown few relationship between \( \text{Qopt} \# \text{QP} \) and \( \# \text{QP} \) except for the trivial inclusion \( \# \text{QP} \subseteq \text{Qopt} \# \text{QP} \). To fill in the gap between them, we begin with a simple observation using Lemma 5.2(4) (see also [30]).
Proposition 7.1 For any function \( h \) in Qopt\(#\)QP, there exists a function \( g \in \#\)QP and a polynomial \( p \) such that, for all strings \( x \) and integers \( m > 0 \),
\[
g(x01^m) \leq h^m(x) \leq 2^p(|x|)g(x01^m).
\]

Proof. Let \( h \) be any function in Qopt\(#\)QP. Let \( h'((x, y)) = h(x)|y| \). By Lemma 5.2(4), \( h' \) belongs to Qopt\(#\)QP. The key idea comes from the fact that, in the proof of Lemma 5.2(4), we can assume that, for a certain fixed polynomial \( p \) and a function \( f \in \#\)QP, \( h'(\langle x, y \rangle) = \sup\{f(\langle x, y \rangle, |\phi|) : |\phi| \) is a qustring of size \( p(|x|) \} \) for all \( x \) and \( y \). Notice that the size of \( |\phi| \) is independent of \( y \).

The rest of the proof is to estimate \( h'((x, y)) \). Define \( g(x01^m) = 2^{-p(|x|)}\sum_{s:|s|=p(|x|)} f(\langle x, 1^m \rangle, s) \) for all \( x \) and \( m \). Obviously, \( g \in \#\)QP. By the maximality of \( h' \), \( f(\langle x, 1^m \rangle, s) \leq h'(\langle x, 1^m \rangle) \) for every \( s \in \Sigma^p(|x|) \). Since the value \( 2^{-p(|x|)}\sum_{s:|s|=p(|x|)} f(\langle x, 1^m \rangle, s) \) is the average of all \( f(\langle x, 1^m \rangle, s) \), we have \( 2^{-p(|x|)}\sum_{s:|s|=p(|x|)} f(\langle x, 1^m \rangle, s) \leq h'(\langle x, 1^m \rangle) \), which implies \( g(x01^m) \leq h'(\langle x, 1^m \rangle) \). On the other hand, \( h'(\langle x, 1^m \rangle) \leq \sum_{s:|s|=p(|x|)} f(\langle x, 1^m \rangle, s) \), which implies \( h'(\langle x, 1^m \rangle) \leq 2^p(|x|)g(x01^m) \). \( \square \)

Although Proposition 7.1 is a rough approximation, it is used as a tool in Section 8.

We further explore a relationship between Qopt\(#\)QP and \#\)QP. In the previous section, we have introduced the notations \( \mathcal{E}_k \) and \( \mathcal{A}_k \) in connection to universal problems. These notations are used to indicate a certain notion of “closeness” (that is, bounded by reciprocal of a polynomial). In this section, we need a much tighter notion of “closeness.”

Definition 7.2 Let \( \mathcal{F} \) and \( \mathcal{G} \) be any two classes of functions. For any function \( f \), we write \( f \mathbin{\mathcal{E}}_e \mathcal{F} \) if, for every polynomial \( p \), there exists a function \( g \in \mathcal{F} \) such that, for every \( x \), \( |f(x) - g(x)| \leq 2^{-p(|x|)} \). The notation \( \mathcal{F} \subseteq_e \mathcal{G} \) means that \( f \mathbin{\mathcal{E}}_e \mathcal{G} \) for all functions \( f \) in \( \mathcal{F} \).

In Proposition 7.4, we show that any quantum optimization problem in Qopt\(#\)QP can be closely approximated by \#\)QP-functions with the help of certain oracles. For this purpose, we define the new class, called QQP. The following definition resembles the \#\)QP-characterization of PP sets in Lemma 3.4.

Definition 7.3 A set \( A \) is in QQP (“quantum optimization polynomial time”) if there exist two functions \( f, g \in \text{Qopt}\#\text{QP} \) and a function \( h \in \text{FPSPACE} \) such that, for every \( x \), \( x \in A \) exactly when \( [2^{|h(x)|}]f(x) > [2^{|h(x)|}]g(x) \). This \( h \) is called a selection function.

Note that, in Definition 7.3, we can replace the value \( |h(x)| \) by \( p(|x|) \) for an appropriate polynomial \( p \). This is seen by taking \( p \) that satisfies \( |h(x)| \leq p(|x|) \) for all \( x \) and by replacing \( f \) and \( g \), respectively, with \( \hat{f}(x) = 2^{-p(|x|)+|h(x)|}f(x) \) and \( \hat{g}(x) = 2^{-p(|x|)+|h(x)|}g(x) \). It also follows from Proposition 3.3 that PP \( \subseteq \text{QQP} \).

In the following proposition, we view an FPSPACE-function as a function from \( \Sigma^* \) to \( \mathbb{D} \).

Proposition 7.4 Qopt\(#\)QP \( \subseteq_e \#\)QP\text{QQP} \( \subseteq_e \text{FPSPACE} \cap D^{\Sigma^*} \).

Proof. Let \( f \in \text{Qopt}\#\text{QP} \). Take a function \( g \in \#\text{QP} \) and a polynomial \( q \) such that \( f(x) = \sup\{g(x, |\phi|) : |\phi| \) is any qustring of size \( q(|x|) \} \) for every \( x \). Define the sets \( A_+ \) and \( A_- \) as follows:
\[
A_+ = \{ (x, y) | 2^q(|x|)+1f(x) \geq \text{num}(y) \}, \quad A_- = \{ (x, y) | 2^q(|x|)+1f(x) \leq \text{num}(y) \},
\]
where \( \text{num}(y) \) is the number \( n \) in \( \mathbb{N} \) such that \( y \) is the \( n \)th string in the standard order (the empty string is the 0th string). Let \( A = A_+ \oplus A_- \), where \( \oplus \) is the disjoint union. It is not difficult to show that \( A \in \text{QQP} \). Let \( p \) be any polynomial. By a standard binary search algorithm using \( A \), we can find an approximation of \( f(x) \) to within \( 2^{-p(|x|)} \) in polynomial time. Let \( h^A \) be the function computed by this algorithm with oracle \( A \). Then, we have \( |f(x) - h^A(x)| \leq 2^{-p(|x|)} \).

For the second inclusion, it suffices to show that Qopt\(#\)QP \( \subseteq_e \text{FPSPACE} \cap D^{\Sigma^*} \) since this implies QQP \( \subseteq \text{PSPACE} \) together with the fact that \#\)QP \( \subseteq_e \text{FPSPACE} \cap D^{\Sigma^*} \) (which follows
from the result in [33]). Let $f$ be any function in $\text{Qopt} \# \text{QP}$. Let $M$ be a QTM that witnesses $f$ with a polynomial $p$ bounding the quantum index size. Recall the QTM $N_{M,p}$ and its associated matrices \{$P_{M,p,x}$\}$_{x \in \Sigma^*}$ given in Section 3 such that, for every $x$, (i) $P_{M,p,x}$ is a $2^{|p(x)|} \times 2^{|p(x)|}$ positive semidefinite, contractive, Hermitian matrix and (ii) $f(x) = \| P_{M,p,x} \|$.

Note that each $(s,t)$-entry of $P_{M,p,x}$ is approximated to within $2^{-m}$ deterministically using space polynomial in $m$, $|x|$, $|s|$, and $|t|$ by simulating all computation paths of $N_{M,p}$ on input $(x,t)$. Consider the characteristic polynomial $u(z) = \det(zI - V)$. This $u(z)$ has the form $u(z) = \sum_{i=0}^{2^{|p(x)|}} a_i z^i$. It is easy to see that each coefficient $a_i$ can be approximated using polynomial space (see also the argument in [31]). Thus, we can also approximate each real root of $u(z)$ using polynomial space. Finally, we find a good approximation of the maximal eigenvalue of $P_{M,p,x}$. Thus, $f \overset{\text{e}}{\in} \text{pFPSPACE} \cap \mathbb{D}^{\Sigma^*}$.

The following is an immediate consequence of Proposition 3.4.

**Corollary 7.5** If $\text{EQP} = \text{QOP}$, then $\text{Qopt} \# \text{QP} \in^e \# \text{QP}$.

The converse of Corollary 7.5 does not seem to hold. Instead, we show the following weaker form of the converse. For our proposition, let $\overline{\text{QOP}}$ denote the subset of $\text{QOP}$ with the extra condition that $|2^{|h(x)|} f(x)| \neq |2^{|h(x)|} g(x)|$ for all $x$ in Definition 3.3.

**Proposition 7.6** If $\text{Qopt} \# \text{QP} \in^e \# \text{QP}$, then $\overline{\text{QOP}} = \text{PP}$ and $\text{QOP} \subseteq \text{P} \# \text{P}^{[1]}$, where $[-]$ stands for the number of queries on each input.

**Proof.** Assume that $\text{Qopt} \# \text{QP} \in^e \# \text{QP}$. We first show that $\overline{\text{QOP}} = \text{PP}$. Let $A$ be any set in $\overline{\text{QOP}}$. There exist a polynomial $p$ and functions $f$ and $g$ in $\text{Qopt} \# \text{QP}$ such that, for every $x$, (i) if $x \in A$ then $|2^{|p(x)|} f(x)| > |2^{|p(x)|} g(x)|$ and (ii) if $x \notin A$ then $|2^{|p(x)|} f(x)| < |2^{|p(x)|} g(x)|$. Since $f \overset{\text{e}}{\in} \text{p}\#\text{QP}$ by our assumption, there exists a certain function $\hat{f}$ in $\#\text{QP}$ such that, for every $x$, $|f(x) - \hat{f}(x)| \leq 2^{-p(|x|)-1}$, which implies that $|2^{|p(x)|} \hat{f}(x)| = |2^{|p(x)|} f(x)|$. Similarly, we obtain $\hat{g}$ from $g$. Assume that $x \in A$. Then, we have $|2^{|p(x)|} \hat{f}(x)| > |2^{|p(x)|} \hat{g}(x)|$. This clearly implies $\hat{f}(x) > \hat{g}(x)$. Similarly, if $x \notin A$ then $\hat{f}(x) < \hat{g}(x)$. Therefore, $A = \{x \mid \hat{f}(x) > \hat{g}(x)\}$. By Lemma 3.4, $A$ belongs to $\text{PP}$.

Next, we show that $\text{QOP} \subseteq \text{P} \# \text{P}^{[1]}$. Let $A$ be in $\text{QOP}$. Similar to 1), we obtain $\hat{f}$ and $\hat{g}$ in $\#\text{QP}$. For this $\hat{f}$, by [33], there exist two functions $\hat{f} \in \text{GapP}$ and $\ell \in \text{FP}$ such that, for every $x$, $|\hat{f}(x) - \hat{g}(x)/\ell(1^{|x|})| \leq 2^{-p(|x|)-1}$. Thus, $|2^{|p(x)|} \hat{f}(x)|$ coincides with the first $p(|x|)$ bits of the binary expansion of $2^{|p(x)|} \hat{f}(x)/\ell(1^{|x|})$. Similarly, we obtain $\hat{g}$ and $\ell'$. Without loss of generality, we can assume that $\ell' = \ell$. To determine whether $x$ is in $A$, we first compute the value $\hat{f}(x)$ and $\hat{g}(x)$ and then compare the first $p(|x|)$ bits of the binary expansion of $2^{|p(x)|} \hat{f}(x)/\ell(1^{|x|})$ and those of $2^{|p(x)|} \hat{g}(x)/\ell(1^{|x|})$. This is done by making one query to each of $\hat{f}$ and $\hat{g}$. It is easy to reduce these two queries to one single query; for example, we can define another $\#\text{P}$-function $h(x)$ to be $2^{|p(x)|} \hat{f}(x) + \hat{g}(x)$, where $q$ is a polynomial satisfying $|\hat{f}(x)| + |\hat{g}(x)| \leq q(|x|)$ for all $x$. Thus, $A$ belongs to $\text{P} \# \text{P}^{[1]}$.

By a simple argument, we next show that $\text{BQP} \neq \text{QMA}$ implies $\text{Qopt} \# \text{QP} \not\in^P \# \text{QP}$. We use the result from Lemma 5.2 (2) that $A \in \text{QMA}$ iff there exists a $f \in \text{Qopt} \# \text{QP}$ such that, for every $x$, if $x \in A$ then $f(x) \geq 3/4$ and otherwise $f(x) \leq 1/4$.

**Lemma 7.7** $\text{Qopt} \# \text{QP} \not\in^P \# \text{QP}$ unless $\text{BQP} = \text{QMA}$.

**Proof.** Assume that $\text{Qopt} \# \text{QP} \in^P \# \text{QP}$. Let $A$ be any set in $\text{QMA}$. Using the amplification property of $\text{QMA}$ (see [21]), we can assume the existence of a function $f$ in $\text{Qopt} \# \text{QP}$ such that, for every $x$, if $x \in A$ then $f(x) \geq 7/8$ and otherwise $f(x) \leq 1/8$. By our assumption, there exists a function $g \in \#\text{QP}$ such that $|f(x) - g(x)| \leq 1/8$. Thus, if $x \in A$ then $g(x) \geq f(x) - \frac{1}{8} \geq \frac{3}{4}$. If $x \notin A$
then \( g(x) \leq f(x) + \frac{1}{8} \leq \frac{1}{2} \). Therefore, \( A \) belongs to BQP.

Recall the fact that \( \text{NP}^A \nsubseteq \text{BQP}^A \) for a certain set \( A \) and that \( \text{NP}^B \subseteq \text{QMA}^B \) for any set \( B \). As a consequence, we obtain the following corollary since Lemma 7.7 relativizes.

**Corollary 7.8** There exists a set \( B \) such that \( \text{Qopt}^\# \text{QP}^B \nsubseteq \text{P}^\# \text{QP}^B \).

## 8 Qopt\#QP-Definable Classes

This section discusses the relationship between quantum optimization problems and known complexity classes. To describe the relationship, one useful notion is “definability” of Fenner et al. [11], which is originally defined only for GapP-functions. The \#QP-definability is also discussed in [33]. We give this “definability” below in a general fashion.

**Definition 8.1** Let \( \mathcal{F} \) be any set of functions from \( \Sigma^* \) to \( \mathbb{R} \). A class \( \mathcal{C} \) of sets is said to be \((\text{uniformly}) \mathcal{F}\text{-definable}\) if there exist an positive integer \( k \) and a pair of disjoint sets \( A, R \subseteq \Sigma^* \times \mathbb{R} \) such that, for every set \( A \) in \( \mathcal{C} \), there exists a function \( f \) in \( \mathcal{F} \) satisfying the following condition: for every \( x \), if \( x \in A \) then \((x, f(x)) \in A \) and otherwise \((x, f(x)) \in R \).

In what follows, we focus on Qopt\#QP-definable classes. Obvious examples of such classes are EQMA and QMA, where EQMA is an error-free restriction of QMA [13] defined as follows. A set \( S \) is in EQMA if there exists a polynomial \( p \) and a polynomial-time \( \mathcal{C} \)-amplitude well-formed QTM \( M \) such that, for every \( x \), (i) if \( x \in S \) then there exists a qustring \( |\phi_x\rangle \) of size \( p(|x|) \) that forces \( M \) to accept \(|x|\langle\phi_x\rangle\) with certainty and (ii) if \( x \notin S \) then, for any qustring \( |\phi\rangle \) of size \( p(|x|) \), \( M \) rejects \(|x|\langle\phi\rangle\) with certainty.

**Lemma 8.2** 1. EQMA is Qopt\#QP-definable. More precisely, \( A \in \text{EQMA} \) iff \( \chi_A \in \text{Qopt}^\# \text{QP} \), where \( \chi_A \) is the characteristic function of \( A \); that is, \( \chi_A(x) = 1 \) if \( x \in A \) and \( \chi_A(x) = 0 \) otherwise.

2. QMA is Qopt\#QP-definable. More strongly, a set \( S \) is in QMA iff there exist a polynomial \( p \) and a function \( f \in \text{Qopt}^\# \text{QP} \) such that, for every \( x \), if \( x \in A \) then \( f(x) \geq 3/4 \) and otherwise \( f(x) \leq 1/4 \).

A less obvious example of Qopt\#QP-definable class is NQP. This is an immediate consequence of Proposition 7.1.

**Lemma 8.3** NQP is Qopt\#QP-definable. More strongly, a set \( A \) is in NQP iff there exists a function \( f \in \text{Qopt}^\# \text{QP} \) such that, for every \( x \), (i) if \( x \in A \) then \( f(x) > 0 \), and (ii) if \( x \notin A \) then \( f(x) = 0 \).

**Proof.** (If - part) Assume that \( A \) and \( f \) in Qopt\#QP satisfy that, for every \( x, x \in A \) iff \( f(x) > 0 \). By Proposition 7.1, there exists a function \( g \in \# \text{QP} \) such that, for every \( x, f(x) > 0 \) iff \( g(x) > 0 \). Thus, \( A \in \text{NQP} \). (Only if - part) This is trivial because \( \# \text{QP} \subseteq \text{Qopt}^\# \text{QP} \).

The class PP is one of the most important complexity classes and PP also contains most well-known quantum complexity classes, such as BQP, QMA, and NQP. Moreover, PP is robust in the sense that it equals PP̄, a quantum interpretation of PP [33]. Thus, it is natural to ask whether PP is Qopt\#QP-definable. The following proposition is a partial answer to this question. This proposition also yields Watrous’s recent result that QMA \( \subseteq \) PP [8].

**Proposition 8.4** Let \( A \) be any subset of \( \{0,1\}^* \). The following statements are equivalent.

1. \( A \) is in PP.
2. For every polynomial \( q \), there exist two functions \( f \in \text{Qopt}^\# \text{QP} \) and \( g \in \text{GapQP} \) such
that, for every string $x$ and integer $m$ ($m \geq |x|$), (i) $g(x01^m) > 0$; (ii) $x \in A$ implies $(1 - 2^{-q(m)})g(x01^m) \leq f(x01^m) \leq g(x01^m)$; and (iii) $x \not\in A$ implies $0 \leq f(x01^m) \leq 2^{-q(m)}g(x01^m)$.

Proof. (1 implies 2) Let $A$ be any set in $\text{PP}$. Note that the following characterization of $\text{PP}$ is well-known (see [22, 14]).

**Fact. 8.5** A set is in $\text{PP}$ iff, for every polynomial $p$, there exist two functions $f, g \in \text{GapP}$ such that, for every $x$ and every $m \geq |x|$, (i) $g(x01^m) > 0$, (ii) $x \in A$ implies $(1 - 2^{-q(m)})g(x01^m) \leq f(x01^m) \leq g(x01^m)$, and (iii) $x \not\in A$ implies $0 \leq f(x01^m) \leq 2^{-q(m)}g(x01^m)$.

Take $\tilde{g}$ and $\tilde{f}$ from $\text{GapQP}$ and $\ell$ from $\text{FP}$ such that $f(x) = \tilde{f}(x)(1^{|x|})$ and $g(x) = \tilde{g}(x)(1^{|x|})$ for all $x$ [33]. We thus replace $g$ and $f$ in Fact 8.5 by $\tilde{g}$ and $\tilde{f}$ and then make all the terms squared. Note that $\tilde{f}^2$ and $\tilde{g}^2$ belong to $\#\text{QP}$ [33] and thus, the both are in $\text{Qopt}\#\text{QP}$. Since $(1 - 2^{-q(m)})^2 \geq 1 - 2^{-q(m)+1}$ and $(2^{-q(m)})^2 \leq 2^{-q(m)+1}$, we can obtain the desired result.

(2 implies 1) Set $q(n) = n$ and assume that there exist two functions $f \in \text{Qopt}\#\text{QP}$ and $g \in \text{GapQP}$ satisfying the conditions of statement 2). Since $g \in \text{GapQP}$ implies $g^2 \in \#\text{QP}$ [33], we can assume from the beginning of this proof that $g \in \#\text{QP}$. For each $x$, let $\hat{x} = x01^{|x|}$. Proposition 7.1 guarantees the existence of a polynomial $p$ and a function $h \in \#\text{QP}$ satisfying that, for every $x$ and $m > 1$, $h(\hat{x}01^m) \leq f^m(\hat{x}) \leq 2^n(\hat{x})h(\hat{x}01^m)$. We can also assume that $p(n) \geq 2$ for all $n \in \mathbb{N}$. Let $g'(x) = 2^{-2p(|x|)}g(|x|)h(\hat{x}01^{|x|})$ and $h'(x) = h(\hat{x}01^{|x|})$ for all $x$. It is easy to see that $g', h' \in \#\text{QP}$ since $g, h \in \#\text{QP}$. In what follows, we show that, for all but finitely-many strings $x, x \in A$ iff $g'(x) < h'(x)$. This implies that, by Lemma 1.4, $A$ is indeed in $\text{PP}$.

Fix $x$ arbitrarily with $n = |x| \geq 4$. In the case where $x \in A$, we obtain:

$$2^{-\frac{p(n)}{n-2}}g^p(n)(\hat{x}) \leq (1 - 2^{-n})^p(n)g^p(n)(\hat{x}) \leq f^p(n)(\hat{x}) \leq 2^n(\hat{x})h(\hat{x}01^p(n))$$

since $(1 - 2^{-n})^p(n) = ((1 - 2^{-n})^{n-2})^{\frac{p(n)}{n-2}}$ and $(1 - 2^{-n})^{n-2} \geq 1 - 2^{-(n-2)+1} = \frac{1}{2}$. This yields the inequality $2^{-p(n)(1+1/(n-2))}g^p(n)(\hat{x}) \leq h'(x)$, which further implies that $g'(x) < h'(x)$ since $n \geq 4$. Consider the other case where $x \not\in A$. In this case, we obtain:

$$h'(x) = h(\hat{x}01^p(n)) \leq f^p(n)(\hat{x}) \leq (2^{-n}p(n))g^p(n)(\hat{x}) \leq 2^{-np(n)}g^p(n)(\hat{x}),$$

which implies $h'(x) < 2^{-2p(n)g^p(n)(\hat{x})} = g'(x)$ since $n > 2$.

\[\square\]

## 9 Complexity Classes Induced from $\text{Qopt}\#\text{QP}$

The $\text{Qopt}\#\text{QP}$-definability is a tool in demonstrating a close relationship between $\text{Qopt}\#\text{QP}$ and other complexity classes. Here, we take another approach toward the study of the complexity of quantum optimization problems. Instead of $\text{Qopt}\#\text{QP}$, we explore complexity classes induced from $\text{Qopt}\#\text{QP}$. We have already seen the class $\text{QOP}$, which has played an important role in approximating quantum optimization problems in Proposition 7.4. The following claim for $\text{QOP}$ is trivial since $\text{Qopt}\#\text{QP} \circ \text{FP} = \text{Qopt}\#\text{QP}$.

**Lemma 9.1** $\text{QOP}$ is closed downward under polynomial-time many-one reductions.

We next focus on sets with low information, known as low sets, for $\text{QOP}$. Here is a general definition of $\mathcal{F}$-low sets.

**Definition 9.2** Let $\mathcal{F}$ be any class (of functions or sets). For any set $A$, $A$ is low for $\mathcal{F}$ (or $\mathcal{F}$-low) if $\mathcal{F}^A = \mathcal{F}$. Let $\text{low-}\mathcal{F}$ denote the collection of all sets that are $\mathcal{F}$-low.
An example of such a low set is \texttt{low-#QP = low-GapQP = EQP} \cite{Li2002}. In the following proposition, we show the low sets for \texttt{Qopt#QP} and \texttt{QOP}.

**Proposition 9.3** 1. \texttt{EQP} \subseteq \texttt{low-Qopt#QP} \subseteq \texttt{EQMA}.
2. \texttt{low-Qopt#QP} \subseteq \texttt{low-QOP} \subseteq \texttt{QOP} \cap \texttt{co-QOP}.

**Proof.** 1) For the first inclusion, assume that \( A \in \texttt{EQP} \). Let \( M_A \) be its associated QTM. Using the squaring lemma in \cite{Li2002}, we can assume that \( M_A \) reaches a specific final configuration (in which the tape content is either \(|x\rangle|1\rangle\) or \(|x\rangle|0\rangle\) and empty elsewhere) with probability 1. Consider any function \( f \) in \texttt{Qopt#QP} and its associated QTM \( M \). As shown in \cite{Li2002}, we can also assume that we have the same number of queries on each computation path of \( M \). We then obtain a non-relativized QTM by substitute the simulation of \( M_A \) for a query given by \( M \). Since this new machine witnesses \( f \), \( f \) belongs to \texttt{Qopt#QP}.

For the second inclusion, assume that \texttt{Qopt#QP} \( A = \texttt{Qopt#QP} \). Since \( \chi_A \in \texttt{Qopt#QP} \), we conclude that \( \chi_A \in \texttt{Qopt#QP} \), which implies that \( A \in \texttt{EQMA} \) by Lemma 8.2(1).

2) The first inclusion is trivial. The second inclusion comes from the fact that \( A \in \texttt{QOP} \cap \texttt{co-QOP} \) for all \( A \).

The difference between \texttt{low-Qopt#QP} and \texttt{low-QOP} stems from the floor-operation (rounding down the terms \( 2^{|h(x)|}f(x) \) and \( 2^{|h(x)|}g(x) \)) for \texttt{QOP} in Definition 7.3.

Another example of \texttt{Qopt#QP}-related class comes from Proposition 8.4. Our complexity class is inspired by Li’s earlier work. Li \cite{Li2002} introduced the complexity class \texttt{APP}: a set \( A \) is in \texttt{APP} ("amplified" \texttt{PP}) iff, for every polynomial \( p \), there exist two functions \( f, g \in \texttt{GapP} \) such that, for every \( x \) and every \( m \geq |x| \), (i) \( g(1^m) > 0 \); (ii) if \( x \in A \) then \( (1 - 2^{-q(m)})g(1^m) \leq f(x01^m) \leq g(1^m) \); and (iii) if \( x \notin A \) then \( 0 \leq f(x01^m) \leq 2^{-q(m)}g(1^m) \). Now, we introduce its quantum extension using \texttt{Qopt#QP}.

**Definition 9.4** A set \( A \) is in \texttt{AQMA} ("amplified" \texttt{QMA}) if, for every polynomial \( q \), there exist two functions \( f \in \texttt{Qopt#QP} \) and \( g \in \texttt{GapQP} \) such that, for every string \( x \) and integer \( m \) (\( m \geq |x| \)),

i) \( g(1^m) > 0 \);

ii) if \( x \in A \) then \((1 - 2^{-q(m)})g(1^m) \leq f(x01^m) \leq g(1^m) \); and

iii) if \( x \notin A \) then \( 0 \leq f(x01^m) \leq 2^{-q(m)}g(1^m) \).

As shown in the proof of Proposition 8.4, by squaring formulas (i) and (ii) in Definition 7.3 (as well as choosing \( q(m) + 1 \)), we can replace the class \texttt{GapQP} by \texttt{#QP}.

Similar to \texttt{APP}, the class \texttt{AQMA} also enjoys simple closure properties: intersection and disjoint union.

**Lemma 9.5** \texttt{AQMA} is closed under intersection and disjoint union.

**Proof.** Let \( A_1 \) and \( A_2 \) be any two sets in \texttt{AQMA}. Also let \( q \) be any polynomial. For each \( i \in \{1, 2\} \), there exist two functions \( f_i \in \texttt{Qopt#QP} \) and \( g_i \in \texttt{GapQP} \) such that, for every \( x \) and \( m \geq |x| \),

i) if \( x \in A_i \) then \((1 - 2^{-q(m)})g_i(1^m) \leq f_i(x01^m) \leq g_i(1^m) \) and

ii) if \( x \notin A_1 \cap A_2 \) then \( 0 \leq f_i(x01^m) \leq 2^{-q(m)}g_i(1^m) \).

By the remark after Definition 7.3, we can assume that \( g_1, g_2 \in \texttt{#QP} \).

For the intersection, note that (i’) if \( x \in A_1 \cap A_2 \) then \((1 - 2^{-q(m)})g_1(1^m)g_2(1^m) \leq f_1(x01^m)f_2(x01^m) \leq g_1(1^m)g_2(1^m) \) and (ii’) if \( x \notin A_1 \cap A_2 \) then \( 0 \leq f_1(x01^m)f_2(x01^m) \leq (2^{-q(m)})^2g_1(1^m)g_2(1^m) \). We define \( g(z) = g_1(z)g_2(z) \) and \( f(z) = f_1(z)f_2(z) \). Obviously, \( g \in \texttt{GapQP} \) and \( f \in \texttt{Qopt#QP} \). Moreover, \((1 - 2^{-q(m)})^2 \geq 1 - 2^{-q(m)+1} \) and \((2^{-q(m)})^2 \leq 2^{-q(m)+1} \). Thus, it suffices to take \( q(m) + 1 \) for \( q(m) \) in (i) and (ii).
For the disjoint union, we first multiply the formulas in both (i) and (ii) by \( g_i(1^m) \), where \( i = 3 - i \). Define \( g(z) = g_1(z)g_2(z) \) for all \( z \). Obviously, \( g \) is in \( \#\text{QP} \). Also, define \( f' \) and \( f'' \) so that \( f'(x1^m) = f_1(x1^m)g_2(1^m) \) and \( f''(x1^m) = g_1(1^m)f_2(x1^m) \). Clearly, \( f', f'' \in \text{Qopt}\#\text{QP} \) since \( g_1, g_2 \in \text{QP} \subseteq \text{Qopt}\#\text{QP} \). Let \( M \) and \( M' \) be appropriate QTMs that witness \( f' \) and \( f'' \), respectively, with a polynomial \( p \) bounding the size of quantum indices. Consider the following QTM \( M \): on input \((bx, |\phi\rangle)\), where \( b \in \{0, 1\} \), \( x \in \Sigma^* \), and \( |\phi\rangle \) is any quantum index of size \( p(|x| + 1) \), if \( b = 0 \) then simulate \( M' \) on input \((x, |\phi\rangle)\); otherwise, simulate \( M'' \) on input \((x, |\phi\rangle)\). Let \( f(z) \) be the maximal acceptance probability, over all \( |\phi\rangle \), of \( M \) on input \((x, |\phi\rangle)\). It is easy to show that \( g \) and \( f \) witness \( A_1 \oplus A_2 \).

The relationships among aforementioned complexity classes are summarized as follows. Watrous’s recent result \( \text{QMA} \subseteq \text{PP} \) is also improved to \( \text{QMA} \subseteq \text{AQMA} \).

**Proposition 9.6** \( \text{APP} \cup \text{QMA} \subseteq \text{AQMA} \subseteq \text{PP} \subseteq \text{QOP} \subseteq \text{PSPACE} \).

**Proof.** It is easy to show that \( \text{APP} \subseteq \text{AQMA} \). We next show that \( \text{QMA} \subseteq \text{AQMA} \). Let \( A \) be any set in \( \text{QMA} \). Note that \( \text{QMA} \) enjoys the amplification property. Let \( q \) be any (nondecreasing) polynomial. There exists a function \( f \in \text{Qopt}\#\text{QP} \) such that, for every \( x \), if \( x \in A \) then \( f(x) \geq 1 - 2^{-q(|x|)} \) and otherwise \( f(x) \leq 2^{-q(|x|)} \). Define \( g(x) = 1 \) for all strings \( x \). It follows that \( f \) and \( g \) satisfy Definition 9.4. The inclusion \( \text{AQMA} \subseteq \text{PP} \) easily follows from Proposition 8.4. Finally, we show that \( \text{PP} \subseteq \text{QOP} \). This is obvious by Lemma 8.4 and the following fact: for every \( f \in \#\text{QP} \), there exists a polynomial \( p \) such that \( |2^{p(|x|)}f(x)| = 2^{p(|x|)}f(x) \) for all \( x \). The last inclusion \( \text{QOP} \subseteq \text{PSPACE} \) follows from Proposition 7.4. □

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**References**

[1] L. M. Adleman, J. DeMarrais, and M. A. Huang, Quantum computability, *SIAM J. Comput.* 26 (1997), 1524–1540.

[2] L. Babai, Trading group theory for randomness, in *Proceedings of the 17th ACM Symposium on Theory of Computing*, pp.421–429, 1985.

[3] C. H. Bennett, E. Bernstein, G. Brassard, and U. Vazirani, Strengths and weaknesses of quantum computing, *SIAM J. Comput.* 26, 1510–1523, 1997.

[4] E. Bernstein and U. Vazirani, Quantum complexity theory, *SIAM J. Comput.* 26, 1411–1473, 1997.

[5] A. Berthiaume, W. van Dam, and S. Laplante, Quantum Kolmogorov complexity, to appear in *J. Comput. System Sci.* See also LANL [quant-ph/0005018] 2000.

[6] H. Buhrman and W. van Dam, Quantum bounded query complexity, in *Proceedings of the 14th Annual Conference on Computational Complexity*, pp.149–157, 1999.

[7] H. Buhrman, J. Kadin, and T. Thierauf, Functions computable with nonadaptive queries to NP, *Theory of Computing Systems*, 31 (1998), 77–92.

[8] Z. Chen and S. Toda, On the complexity of computing optimal solutions, *International Journal of Foundations of Computer Science* 2 (1991), 207–220.
[9] D. Deutsch, Quantum theory, the Church-Turing principle, and the universal quantum computer, *Proc. Roy. Soc. London*, A, **400** (1985), 97–117.

[10] D. Du and K. Ko, *Theory of Computational Complexity*, John Wiley & Sons, Inc., 2000.

[11] S. Fenner, L. Fortnow, and S. Kurtz, Gap-definable counting classes, *J. Comput. System Sci.*, **48** (1994), 116–148.

[12] S. Fenner, F. Green, S. Homer, and R. Pruim, Determining acceptance probability for a quantum computation is hard for the polynomial hierarchy, *Proceedings of the Royal Society of London*, Ser. A, **455**, 3953–3966, 1999.

[13] L. Fortnow and J. Rogers, Complexity limitations on quantum computation, *J. Comput. System Sci.*, **59** (1999), 240–252.

[14] L. A. Hemaspandra and M. Ogihara, *The Complexity Theory Companion*, Springer-Verlag, 2002.

[15] R. A. Horn and C. R. Johnson, *Matrix Analysis*, Cambridge University Press, 1985.

[16] A. Kitaev, “Quantum NP”, Public Talk at AQIP’99: 2nd Workshop on Algorithms in Quantum Information Processing, DePaul University, 1999.

[17] A. Kitaev and J. Watrous, Parallelization, amplification, and exponential time simulation of quantum interactive proof systems, in *Proceedings of the 32nd ACM Symposium on Theory of Computing*, pp.608–617, 2000.

[18] H. Kobayashi, K. Matsumoto, and T. Yamakami, Quantum Merlin Arthur proof systems, Los Alamos Archive [quant-ph/0110006] 2001.

[19] J. Köbler, U. Schöning, and J. Torán, On Counting and Approximation, *Acta Informatica*, **26** (1989), 363–379.

[20] M. W. Krentel, The complexity of optimization problems, *J. Comput. System Sci.*, **36** (1988), 490–509.

[21] M. W. Krentel, Generalizations of OptP to the polynomial hierarchy, *Theoretical Computer Science*, **97** (1992), 183–198.

[22] L. Li, On the counting functions, Ph.D. thesis, Department of Computer Science, University of Chicago, 1993. Also see technical report TR 93-12.

[23] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press, 2000.

[24] M. Ogihara and L. Hemachandra, A complexity theory for feasible closure properties, *J. Comput. System Sci.*, **46** (1993), 295–325.

[25] M. Ozawa and H. Nishimura, Local transition functions of quantum Turing machines, in *Proceedings of the 4th International Conference on Quantum Communication, Complexity, and Measurement*, 1999.

[26] L. Valiant, The complexity of computing the permanent, *Theor. Comput. Sci.* **8** (1979), 189–201.

[27] P. M. B. Vitányi, Quantum Kolmogorov complexity based on classical descriptions, *IEEE Transactions on Information Theory*, **47** (2001), 2464–2479.

[28] J. Watrous, PSPACE has constant-round quantum interactive proof systems, in *Proceedings of the 40th Annual Symposium on Foundations of Computer Science*, pp.112–119, 1999.

[29] J. Watrous, Succinct quantum proofs for properties of finite groups, in *Proceedings of the 41st Annual Symposium on Foundations of Computer Science*, pp.537–546, 2000.

[30] J. Watrous, Note on simulating QMA in PP, manuscript, August 2001.

[31] J. Watrous, Quantum statistical zero-knowledge, LANL [quant-ph/0202111] 2002.

[32] T. Yamakami, A foundation of programming a multi-tape quantum Turing machine, in Proceedings of the 24th International Symposium on Mathematical Foundation of Computer Science, Lecture Notes in Computer Science, Vol.1672, pp.430–441, 1999.

[33] T. Yamakami, Analysis of quantum functions, in Proceedings of the 19th International Conference on Foundations of Software Technology and Theoretical Computer Science, Lecture Notes in Computer Science, Vol.1738, pp.407–419, 1999. A journal revision, manuscript, 2002.

[34] T. Yamakami and A. C. Yao, NQP$^c_{\leq}$ = co-C$^P_{\leq}$, *Inf. Process. Let.* **71** (1999), 63–69.

[35] A. C. Yao, Quantum circuit complexity, in *Proceedings of the 34th Annual Symposium on Foundations of Computer Science*, pp.352–361, 1993.
Appendix

We show from [32] three local requirements on a quantum transition function that its associated QTM should be well-formed.

We begin with the simple case of 1-tape QTMs. Let \( M = (Q, \{q_0\}, Q_f, \Sigma, \delta) \) be a 1-tape QTM with initial state \( q_0 \) and a set \( Q_f \) of final states. As noted before, the head move directions \( R, N, \) and \( L \) are freely identified with \( -1, 0, \) and \( +1, \) respectively. We introduce new notation that is helpful to describe the well-formedness of QTMs. Let \( D = \{0, 1, -1\}, E = \{0, \pm 1, \pm 2\}, \) and \( H = \{0, \pm 1, \pm 2\} \).

For \( d \in D \) and \( \epsilon \in E \), we write \( E_d = \{ \epsilon \in E \mid |2d - \epsilon| \leq 1 \} \) and \( D_\epsilon = \{ d \in D \mid |2d - \epsilon| \leq 1 \} \). Let \((p, \sigma, \tau) \in Q \times \Sigma^2 \) and \( \epsilon \in E \).

Bernstein and Vazirani [4] introduced the notation \( \delta(p, \sigma|\tau, d) \) for \( \sum_{q \in Q} \delta(p, \sigma, q, \tau, d)|q\rangle \). Instead of their notation, we introduce the notation \( \delta[p, \sigma, \tau|\epsilon] \). An element \( \delta[p, \sigma, \tau|\epsilon] \) in \( \mathbb{C}^H \) is defined as:

\[
\delta[p, \sigma, \tau|\epsilon] = \sum_{q \in Q} \frac{\delta(p, \sigma, q, \tau, d)}{|E_d|} |q\rangle h_{d,\epsilon},
\]

where \( h_{d,\epsilon} = 2d - \epsilon \) if \( \epsilon \neq 0 \) and \( h_{d,\epsilon} = \epsilon \) otherwise. The term \( \sqrt{|E_d|} \) in the above equation ensures that \( \sum_{\epsilon \in E} \|\delta[p, \sigma, \tau|\epsilon]\|^2 = \sum_{d \in D} \|\delta(p, \sigma|\tau, d)\|^2 \).

**Lemma 9.7** A 1-tape QTM \( M = (Q, \{q_0\}, Q_f, \Sigma, \delta) \) is well-formed iff the following three conditions hold.

1. (unit length) \( \|\delta(p, \sigma)\| = 1 \) for all \( (p, \sigma) \in Q \times \Sigma \).
2. (orthogonality) \( \delta(p_1, \sigma_1) \cdot \delta(p_2, \sigma_2) = 0 \) for any distinct pair \( (p_1, \sigma_1), (p_2, \sigma_2) \in Q \times \Sigma \).
3. (separability) \( \delta[p_1, \sigma_1, \tau_1|\epsilon] \cdot \delta[p_2, \sigma_2, \tau_2|\epsilon'] = 0 \) for any distinct pair \( \epsilon, \epsilon' \in E \) and for any pair \( (p_1, \sigma_1, \tau_1), (p_2, \sigma_2, \tau_2) \in Q \times \Sigma^2 \).

We return to the case of \( k \)-tape QTMs. Now we expand the notation \( \delta[p, \sigma, \tau|\epsilon] \) as follows. Let \( (p, \sigma, \tau) \in Q \times (\Sigma^k)^2 \) and \( \epsilon \in E^k \). Let \( D_\epsilon = \{ d \in D^k \mid \forall i \in \{1, \ldots, k\} (|2d_i - \epsilon_i| \leq 1) \} \), where \( d = (d_i)_{1 \leq i \leq k} \) and \( \epsilon = (\epsilon_i)_{1 \leq i \leq k} \). Let \( h_{d,\epsilon} = (h_{d_i,\epsilon_i})_{1 \leq i \leq k} \). Note that if \( |\epsilon| \neq |\epsilon'| \) then \( h_{d,\epsilon} \neq h_{d',\epsilon'} \) for any \( d \in D_\epsilon \) and any \( d' \in D_{\epsilon'} \), where \( |\epsilon| = (|\epsilon_i|)_{1 \leq i \leq k} \).

We define \( \delta[p, \sigma, \tau|\epsilon] \) as follows:

\[
\delta[p, \sigma, \tau|\epsilon] = \sum_{q \in Q} \sum_{d \in E_\epsilon} \frac{\delta(p, \sigma, q, \tau, d)}{|E_d|} |q\rangle h_{d,\epsilon}.
\]

Since any two distinct tapes do not interfere, multi-tape QTMs must satisfy the \( k \) independent conditions of Lemma 9.7. Thus, we obtain:

**Lemma 9.8** (Well-Formedness Lemma) Let \( k \geq 1 \). A \( k \)-tape QTM \( M = (Q, \{q_0\}, Q_f, \Sigma^k, \delta) \) is well-formed iff the following three conditions hold.

1. (unit length) \( \|\delta(p, \sigma)\| = 1 \) for all \( (p, \sigma) \in Q \times \Sigma^k \).
2. (orthogonality) \( \delta(p_1, \sigma_1) \cdot \delta(p_2, \sigma_2) = 0 \) for any distinct pairs \( (p_1, \sigma_1), (p_2, \sigma_2) \in Q \times \Sigma^k \).
3. (separability) \( \delta[p_1, \sigma_1, \tau_1|\epsilon] \cdot \delta[p_2, \sigma_2, \tau_2|\epsilon'] = 0 \) for any distinct pair \( \epsilon, \epsilon' \in E^k \) and for any pair \( (p_1, \sigma_1, \tau_1), (p_2, \sigma_2, \tau_2) \in Q \times (\Sigma^k)^2 \).
At the end of this appendix, we give the proof of Lemma 6.6.

**Proof of Lemma 6.6.** Let $ACC$ and $REJ$ be the sets of all accepting configurations and rejecting configurations, respectively. Let $ALL = ACC \cup REJ$. Assume that $U_M |\phi\rangle = \sum_{i \in ALL} \alpha_i |i\rangle$ and $U_N |\psi\rangle = \sum_{i \in ALL} \beta_i |i\rangle$.

$$2|\eta_M(|\phi\rangle) - \eta_N(|\psi\rangle)| = |\eta_M(|\phi\rangle) - \eta_N(|\psi\rangle)| + |\eta_M(|\phi\rangle) - \eta_N(|\psi\rangle)|$$

$$\leq \sum_{i \in ACC} ||\alpha_i|^2 - |\beta_i|^2| + \sum_{i \in REJ} ||\alpha_i|^2 - |\beta_i|^2|$$

$$= \sum_{i \in ALL} |(|\alpha_i| - |\beta_i|)(|\alpha_i| + |\beta_i|)|$$

$$\leq \sum_{i \in ALL} |\alpha_i - \beta_i||\alpha_i| + \sum_{i \in ALL} |\alpha_i - \beta_i||\beta_i|$$

$$\leq \left( \sum_{i \in ALL} |\alpha_i - \beta_i|^2 \sum_{i \in ALL} |\alpha_i|^2 \right)^{1/2} + \left( \sum_{i \in ALL} |\alpha_i - \beta_i|^2 \sum_{i \in ALL} |\beta_i|^2 \right)^{1/2}$$

$$= 2 \left( \sum_{i \in ALL} |\alpha_i - \beta_i|^2 \right)^{1/2}$$

$$= 2\| U_M |\phi\rangle - U_N |\psi\rangle \|_2,$$

where $\eta_M(x)$ is the rejection probability of $M$ on input $x$. For the first and the second inequalities, we use $||\alpha_i| - |\beta_i|| \leq |\alpha_i - \beta_i|$ and the Cauchy-Schwartz inequality. □