A Foundation of Programming a Multi-Tape Quantum Turing Machine

(Preliminary Version)

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Abstract. The notion of quantum Turing machines is a basis of quantum complexity theory. We discuss a general model of multi-tape, multi-head Quantum Turing machines with multi final states that also allow tape heads to stay still.

1 Introduction

A quantum Turing machine (QTM) is a theoretical model of quantum computers, which expands the classical model of a Turing machine (TM) by allowing quantum interference to take place on their computation paths. Designing a QTM in general, however, is significantly harder than that of a classical TM because of its well-formedness condition as well as its halting condition, known as the timing problem. Recently Bernstein and Vazirani [2] initiated a study of quantum complexity theory founded on a restrictive model: a one-head, multitrack, stationary, dynamic, normal form, unidirectional QTM (for definitions, see Section 2) that prohibits a tape head to stay still. We call such a restrictive QTM conservative for convenience.

One may find easier to program a less restrictive QTM when he wishes to solve a problem on a quantum computer. In this paper we wish to introduce a QTM as general as possible. In Section 2, we introduce a multi-tape, multi-head QTM with multi final states that also allows tape heads to stay still. Although many variations of QTMs are known to be polynomially equivalent [2,3], unsolved is the question of what is the degree of polynomials of these simulation overhead. As we will show in Section 4, any multi-tape, multi-head, well-formed QTM can be effectively simulated by a conservative QTM with only cubic polynomial slowdown.

Our primary goal is to contribute to the foundation of programming a handy QTM. In Section 3, we will prove two fundamental lemmas: Well-formedness Lemma and Completion Lemma, which are important tools in constructing a

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QTM. The lemmas expand the results of Bernstein and Vazirani [2], who considered mostly conservative QTMs. Using the lemmas, we will show that any computation of a well-formed QTM can be reversed on a well-formed QTM with quadratic polynomial slowdown. We will also address the timing problem in Section 4. In Section 5, we will focus on an oracle QTM with multi query tapes and multi oracles. For any oracle QTM M, we can build an oracle QTM, similar to the classical case, that simulates M with a fixed number of queries of fixed length on every computation path.

2 Definition of Quantum Turing Machines

This section briefly describes the formal definition of quantum Turing machines. For our purpose, we wish to make the definition as general as possible. Here we present a definition that is slightly more general than the one given in [2,1].

A k-tape quantum Turing machine (QTM) M is a quintuple $(Q, \{q_0\}, Q_f, \Sigma_1 \times \Sigma_2 \times \cdots \times \Sigma_k, \delta)$, where each Σ_i is a finite alphabet with a distinguished blank symbol #, Q is a finite set of internal states including an initial state q_0 and $Q_f = \{q_f^1, q_f^2, \dots, q_k^m\}$, a set of final states, and δ is a multi-valued, quantum transition function from $Q \times \Sigma_1 \times \Sigma_2 \times \cdots \times \Sigma_k$ to $\mathbb{C}^{Q \times \Sigma_1 \times \Sigma_2 \times \cdots \times \Sigma_k \times \{R, N, L\}^k}$. (Note that $\delta(q_f^i, \sigma)$ must be defined.) For brevity, write $\tilde{\Sigma}^{(k)}$ for $\Sigma_1 \times \cdots \times \Sigma_k$. A QTM has two-way infinite tapes of cells indexed by \mathbb{Z} and read/write tape heads that move along the tapes. Directions R and L mean that a head steps right and left, respectively, and direction N mean that a head makes no movement. We say that all tape heads move concurrently if they move in the same direction at any time (in this case, e.g., we write $\delta(p, \sigma, q, \tau, d)$ instead of $\delta(p, \sigma, q, \tau, d)$). We call a QTM dynamic if its heads never stay still. A QTM is unidirectional if, for any $p_1, p_2, q \in Q$, $\sigma_1, \sigma_2 \in \tilde{\Sigma}^{(k)}$, and $d_1, d_2 \in \{L, N, R\}^k$, $\delta(p_1, \sigma_2, q, \tau_1, d_1) \cdot \delta(p_2, \sigma_2, q, \tau_2, d_2) \neq 0$ implies $d_1 = d_2$.

We assume the reader's familiarity with the following terminology: a time-evolution operator, a configuration and final configuration, a superposition and a final superposition, a well-behaved and stationary QTM, and the acceptance probability of a QTM. For their definitions, see [2].

Here are ones different from [2]. A QTM is in normal form if, for every $i \in \{1, 2, ..., m\}$, there exists a direction $\mathbf{d}_i \in \{L, N, R\}^k$ such that $\delta(q_f, \boldsymbol{\sigma}) = |q_0\rangle|\boldsymbol{\sigma}\rangle|\mathbf{d}_i\rangle$ for any $\boldsymbol{\sigma} \in \tilde{\Sigma}^{(k)}$. A QTM M is called synchronous if, for every \boldsymbol{x} , any two computation paths of M on \boldsymbol{x} reach final configurations at the same time. The running time of M on \boldsymbol{x} is defined to be the minimal number T such that, at time T, all computation paths of M on \boldsymbol{x} reach final configurations. We write $\mathrm{Time}_M(\boldsymbol{x})$ to denote the running time of M on \boldsymbol{x} if one exists; otherwise, it is undefined. We say that M on input \boldsymbol{x} halts in time T if $\mathrm{Time}_M(\boldsymbol{x})$ exists and $\mathrm{Time}_M(\boldsymbol{x}) = T$. A QTM is well-formed if its time-evolution operator preserves the L_2 -norm. A multi-tape QTM is said to be conservative if it is a well-formed, stationary, dynamic, unidirectional QTM in normal form with concurrent head move. We write $\mu_M(\boldsymbol{x})$ to denote the probability that M accepts input \boldsymbol{x} .

Throughout this paper, T denotes a function from Σ^* to \mathbb{N} .

3 Fundamentals of Quantum Turing Machines

In this section, we will prove two lemmas that are essential tools in programming a well-formed QTM: Well-Formedness Lemma and Completion Lemma.

For convenience, the head move directions R, N, and L are identified with -1, 0, and +1, respectively.

Well-Formedness Lemma. One of the most significant feature of a QTM is the well-formedness condition on its quantum transition function that reflects the unitarity of their corresponding time-evolution operators. Here we present in Lemma 1 three local requirements for a quantum transition function whose associated QTM is well-formed.

Let $M = (Q, \{q_0\}, Q_f, \Sigma_1 \times \cdots \times \Sigma_k, \delta)$ be a k-tape QTM. Recall that $\tilde{\Sigma}^{(k)}$ stands for $\Sigma_1 \times \cdots \times \Sigma_k$. We introduce the notation $\delta[p, \sigma, \tau|\epsilon]$. Let $D = \{0, \pm 1\}$, $E = \{0, \pm 1, \pm 2\}$, and $H = \{0, \pm 1, \natural\}$. Let $(p, \sigma, \tau) \in Q \times (\tilde{\Sigma}^{(k)})^2$ and $\epsilon \in E^k$. Define $D_{\epsilon} = \{d \in D^k \mid \forall i \in \{1, \dots, k\} (|2d_i - \epsilon_i| \le 1)\}$ and $E_{\mathbf{d}} = \{\epsilon \in E^k \mid d \in D_{\epsilon}\}$, where $\mathbf{d} = (d_i)_{1 \le i \le k}$ and $\epsilon = (\epsilon_i)_{1 \le i \le k}$. Let $h_{\mathbf{d}, \epsilon} = (h_{d_i, \epsilon_i})_{1 \le i \le k}$, where $h_{d, \epsilon} = 2d - \epsilon$ if $\epsilon \ne 0$ and $h_{d, \epsilon} = \natural$ otherwise. Finally, we define $\delta[p, \sigma, \tau|\epsilon]$ as follows: $\delta[p, \sigma, \tau|\epsilon] = \sum_{q \in Q} \sum_{\mathbf{d} \in D_{\epsilon}} \delta(p, \sigma, q, \tau, \mathbf{d}) |E_{\mathbf{d}}|^{-1/2} |q\rangle |h_{\mathbf{d}, \epsilon}\rangle$.

Lemma 1. (Well-Formedness Lemma) A k-tape QTM $M = (Q, \{q_0\}, Q_f, \Sigma_1 \times \cdots \times \Sigma_k, \delta)$ is well-formed iff the following three conditions hold.

- 1. (unit length) $\|\delta(p, \boldsymbol{\sigma})\| = 1$ for all $(p, \boldsymbol{\sigma}) \in Q \times \tilde{\Sigma}^{(k)}$.
- 2. (orthogonality) $\delta(p_1, \boldsymbol{\sigma}_1) \cdot \delta(p_2, \boldsymbol{\sigma}_2) = 0$ for any distinct pair $(p_1, \boldsymbol{\sigma}_1), (p_2, \boldsymbol{\sigma}_2) \in Q \times \tilde{\Sigma}^{(k)}$.
- 3. (separability) $\delta[p_1, \boldsymbol{\sigma}_1, \boldsymbol{\tau}_1 | \boldsymbol{\epsilon}] \cdot \delta[p_2, \boldsymbol{\sigma}_2, \boldsymbol{\tau}_2 | \boldsymbol{\epsilon}'] = 0$ for any distinct pair $\boldsymbol{\epsilon}, \boldsymbol{\epsilon}' \in E^k$ and for any pair $(p_1, \boldsymbol{\sigma}_1, \boldsymbol{\tau}_1), (p_2, \boldsymbol{\sigma}_2, \boldsymbol{\tau}_2) \in Q \times (\tilde{\Sigma}^{(k)})^2$.

The proof of the lemma is similar to that of Theorem 5.3 in [2]. Note that, since any two distinct tapes do not interfere, a k-tape QTM must satisfy the k independent conditions for the case k=1. We leave the detail to the reader.

Completion Lemma. A quintuple $M = (Q, \{q_0\}, Q_f, \Sigma_1 \times \cdots \times \Sigma_k, \delta)$ is called a partial QTM if δ is a partial quantum transition function that is defined on a subset S of $Q \times \Sigma_1 \times \cdots \times \Sigma_k$. If δ satisfies the three conditions of Lemma 1 on all entries of δ , then we call M a well-formed partial QTM [2].

Completion Lemma says that any well-formed partial QTM can be expanded to a well-formed QTM.

Lemma 2. (Completion Lemma) For every k-tape, well-formed partial QTM with quantum transition function δ , there exists a k-tape, well-formed QTM with the same state set and alphabet whose transition function δ' agrees with δ whenever δ is defined.

To show the lemma, we first consider how to change the basis of a given QTM. Let $M = (Q, \{q_0\}, Q_f, \Sigma_1 \times \cdots \times \Sigma_k, \delta)$ be a given QTM. We first partition

 $\mathbb{C}^{Q\times H^k} \text{ into mutually orthogonal spaces } \{\mathbb{C}_{\boldsymbol{\epsilon}}\mid \boldsymbol{\epsilon}\in E^k\} \text{ such that (i) } \mathbb{C}^{Q\times H^k} = span\{\mathbb{C}_{\boldsymbol{\epsilon}}\mid \boldsymbol{\epsilon}\in E^k\} \text{ and (ii) for any } \boldsymbol{\epsilon}\in E^k \text{ and any } (p,\boldsymbol{\sigma},\boldsymbol{\tau})\in Q\times (\tilde{\Sigma}^{(k)})^2, \\ \delta[p,\boldsymbol{\sigma},\boldsymbol{\tau}|\boldsymbol{\epsilon}]\in \mathbb{C}_{\boldsymbol{\epsilon}}. \text{ Note that if } |\boldsymbol{\epsilon}|\neq |\boldsymbol{\epsilon}'| \text{ then } \mathbb{C}_{\boldsymbol{\epsilon}}\cap \mathbb{C}_{\boldsymbol{\epsilon'}}=\emptyset. \text{ For each } \boldsymbol{\epsilon}\in E^k, \text{ let } B_{\boldsymbol{\epsilon}} \text{ be an orthonormal basis for } \mathbb{C}_{\boldsymbol{\epsilon}}. \text{ Let } B \text{ be the union of all such } B_{\boldsymbol{\epsilon}}\text{'s.}$

We assume that, at time t, M in state p scans symbol σ and that δ maps (p, σ) to $\sum_{q, \tau, d} \delta(p, \sigma, q, \tau, d) |q\rangle |\tau\rangle |d\rangle$. Define the change of basis from $Q \times \{L, N, R\}^k$ to $B \times E^k$ by mapping $|q\rangle |d\rangle$ into $\sum_{w \in B} \sum_{\epsilon \in E_{\boldsymbol{d}}} \langle h_{\boldsymbol{d}, \epsilon}, q |w\rangle |E_{\boldsymbol{d}}|^{-1/2} |w\rangle |\epsilon\rangle$. Let U_1 denote this transform. This matrix U_1 is unitary because $\langle \boldsymbol{d}, q | U_1^* U_1 | q', \boldsymbol{d}' \rangle = \sum_{\epsilon \in E_{\boldsymbol{d}} \cap E_{\boldsymbol{d}'}} \langle h_{\boldsymbol{d}', \epsilon}, q' | q, h_{\boldsymbol{d}, \epsilon} \rangle (|E_{\boldsymbol{d}}| \cdot |E_{\boldsymbol{d}'}|)^{-1/2} = \langle \boldsymbol{d}, q | q', \boldsymbol{d}' \rangle$, which implies $U_1^* U_1 = I$. It is known in [2] that U_1 preserves the L_2 -norm iff U_1 is unitary.

Let $\delta'(p, \boldsymbol{\sigma})$ denote $U_1\delta(p, \boldsymbol{\sigma})$ for any $(p, \boldsymbol{\sigma}) \in S$. In what follows, we show that δ' is "unidirectional" in the sense that if $\delta'(p, \boldsymbol{\sigma}, v, \boldsymbol{\tau}, \boldsymbol{\epsilon}) \cdot \delta'(p', \boldsymbol{\sigma}', v, \boldsymbol{\tau}', \boldsymbol{\epsilon}') \neq 0$ then $\boldsymbol{\epsilon} = \boldsymbol{\epsilon}'$. Let $\boldsymbol{\epsilon}$ and $\boldsymbol{\epsilon}'$ be distinct and in E^k . Note that the separability condition ensures that $\delta[p, \boldsymbol{\sigma}, \boldsymbol{\tau}|\boldsymbol{\epsilon}] \cdot \delta[p', \boldsymbol{\sigma}', \boldsymbol{\tau}'|\boldsymbol{\epsilon}'] = 0$ for any $(p', \boldsymbol{\sigma}', \boldsymbol{\tau}') \in Q \times (\tilde{\Sigma}^{(k)})^2$. Since $\delta[p, \boldsymbol{\sigma}, \boldsymbol{\tau}|\boldsymbol{\epsilon}] = \sum_{v \in B} \delta'(p, \boldsymbol{\sigma}, v, \boldsymbol{\tau}, \boldsymbol{\epsilon})|v\rangle \in \mathbb{C}_{\boldsymbol{\epsilon}}$, $\delta'(p, \boldsymbol{\sigma}, v, \boldsymbol{\tau}, \boldsymbol{\epsilon}) = 0$ for any $v \in B_{\boldsymbol{\epsilon}'}$ if $\boldsymbol{\epsilon} \neq \boldsymbol{\epsilon}'$. Therefore, δ' is "unidirectional."

The transform U_1 is useful to show Completion Lemma. We go back to the formal proof of Completion Lemma.

Proof of Lemma 2. Let $M = (Q, \{q_0\}, Q_f, \Sigma_1 \times \cdots \times \Sigma_k, \delta)$ be a given QTM. Let U_1 be defined as above. As shown above, U_1 is unitary. As a result, $\delta'(S)$ is a set of orthonormal vectors since so is $\delta(S)$.

For each $v \in B$, let ϵ_v be ϵ such that $\delta'(p, \sigma, v, \tau, \epsilon) \neq 0$ for some $(p, \sigma, \tau) \in Q \times (\tilde{\Sigma}^{(k)})^2$ if any, and let $\epsilon_v = (1)_{1 \leq i \leq k}$ otherwise. Since δ' is "unidirectional", ϵ_v is uniquely determined. This implies that we can define the vector $\delta''(p, \sigma)$ as $\delta''(p, \sigma) = \sum_{v \in B} \sum_{\tau \in \tilde{\Sigma}^{(k)}} \delta'(p, \sigma, v, \tau, \epsilon_v)|v\rangle|\tau\rangle$.

Now we expand δ'' to $Q \times \tilde{\Sigma}^{(k)}$ by adding arbitrarily extra orthonormal vectors associated with elements in $Q \times \tilde{\Sigma}^{(k)} - S$. Let $\overline{\delta}''$ be such an expansion of δ'' . We define $\overline{\delta}'$ by $\overline{\delta}'(p, \boldsymbol{\sigma}) = \sum_{v \in B} \sum_{\boldsymbol{\tau} \in \tilde{\Sigma}^{(k)}} \sum_{\boldsymbol{\epsilon} \in E^k} \overline{\delta}''(p, \boldsymbol{\sigma}, v, \boldsymbol{\tau}, \boldsymbol{\epsilon})|v\rangle |\boldsymbol{\tau}\rangle |\boldsymbol{\epsilon}\rangle$.

We then apply the inverse transform U_1^* to $\overline{\delta}'(Q \times \tilde{\Sigma}^{(k)})$ and let $\overline{\delta}$ be the result obtained. Define $\overline{M} = (Q, \{q_0\}, Q_f, \tilde{\Sigma}^{(k)}, \overline{\delta})$. Since U_1 is unitary, \overline{M} must be well-formed.

Completion Lemma also enables us to use a k-tuple of a single alphabet, Σ^k , instead of $\Sigma_1 \times \ldots \times \Sigma_k$. In the following sections, we will deal only with a k-tape QTM with tape alphabets Σ^k .

4 Simulation of Quantum Turing Machines

In this section we demonstrate several simulation results using the main lemmas in Section 3. Since we are interested only in the acceptance probability of a QTM, the "simulation" of a QTM M by another QTM M' in this paper regards with the statement that N produces the same acceptance probability as M does.

More formally, we say that M' simulates M with slowdown f if, for every \boldsymbol{x} , $\mu_{M'}(\boldsymbol{x}) = \mu_{M}(\boldsymbol{x})$ and $\operatorname{Time}_{M'}(\boldsymbol{x}) = f(\operatorname{Time}_{M}(\boldsymbol{x}))$.

Assume that M is a k-tape well-formed QTM running in time $T(\boldsymbol{x})$ on input \boldsymbol{x} . For $m \geq 1$, let $\tilde{M}_{T,m}$ denote the (k+m)-tape QTM that, on input \boldsymbol{x} in tapes 1 to k and $1^{T(\boldsymbol{x})}$ in tape k+1 and empty elsewhere, behaves like M on input \boldsymbol{x} except that the heads in tapes k+1 to k+m idle in the start cells. The tape alphabets of $\tilde{M}_{T,m}$ for tapes 1 to k are the same as M's.

For convenience, let $M(|\phi\rangle)$ denote the final superposition of M that starts with superposition $|\phi\rangle$. In the case where $|\phi\rangle$ is an initial configuration with input \boldsymbol{x} , we write $M(|\boldsymbol{x}\rangle)$ for $M(|\phi\rangle)$.

For any pair $\boldsymbol{\sigma} = (\sigma_i)_{1 \leq i \leq k}$ and $\boldsymbol{\tau} = (\tau_j)_{1 \leq j \leq m}$, $\boldsymbol{\sigma} * \boldsymbol{\tau}$ denotes the (k+m)-tuple $(\sigma_1, \ldots, \sigma_k, \tau_1, \ldots, \tau_m)$. In particular, we write $s * \boldsymbol{\sigma}$ for $(s) * \boldsymbol{\sigma}$ and $\boldsymbol{\sigma} * s$ for $\boldsymbol{\sigma} * (s)$.

Simulation by Synchronous Machines. We show how to transform any well-formed QTM into a well-formed, synchronous QTM with a single final state with the help of the information on its running time.

Lemma 3. Let M be a k-tape, well-formed QTM that halts in time $T(\mathbf{x})$ on any k-tuple input string \mathbf{x} . Then, there exists a (k+2)-tape, well-formed, synchronous QTM M' with a single final state such that, on input $(\mathbf{x}, 1^{T(\mathbf{x})})$, it halts in time $2T(\mathbf{x}) + 2$, the last two tape heads move back to the start cells, leaving $1^{T(\mathbf{x})}$ unchanged, and $\mu_{M'}(\mathbf{x}, 1^{T(\mathbf{x})}) = \mu_{M}(\mathbf{x})$. If M already has a single final state, then M' needs only k+1 tapes and satisfies $M'(|\mathbf{x}, 1^{T(\mathbf{x})}\rangle) = \tilde{M}_{T,1}(|\mathbf{x}, 1^{T(\mathbf{x})}\rangle)$.

Proof. Let $M = (Q, \{q_0\}, Q_f, \Sigma^k, \delta)$ be a given QTM with $Q_f = \{q_f^1, q_f^2, \dots, q_f^m\}$. By Completeness Lemma, it suffices to build a partial QTM M' that satisfies the lemma. Assume that \boldsymbol{x} is given in tapes 1 to k and $1^{T(\boldsymbol{x})}$ is in tape k+1. Tape k+2 is initially empty. The QTM M' simulates each step of the computation of M using tapes 1 to k, together with stepping right in tape k+1, which counts the number of steps executed by M. When M' arrives at any final configuration of M with final state q_f^i , $1 \leq i \leq m$, at time exactly $T(\boldsymbol{x})$, M' deposits the number i (as a single tape symbol) onto tape k+2, freeing itself from state q_f^i . Then, M' moves its k+1st tape head back to the start cell in $T(\boldsymbol{x})+2$ steps and enters its own final state q_f . Thus, the running time of M' is exactly $2T(\boldsymbol{x})+2$.

It is not difficult to check the well-formedness of M' using Well-Formedness Lemma. Note that the acceptance probability of M does not change during the above simulation process. Thus, $\mu_{M'}(1^{T(\boldsymbol{x})}, \boldsymbol{x}) = \mu_{M}(\boldsymbol{x})$.

If M already has a single final state q_f , we modify the above procedure in the following fashion. Firstly, we replace every occurrence of q_f in δ by \hat{q}_f . Secondly, we apply the above simulation procedure. Thirdly, after the simulation, we force M' to enter q_f as its final state exactly when the k+1st tape head returns to the start cell. In this case, we do not need the k+2nd tape at all.

Simulation by Machines with Concurrent Head Move. The simulation of a multi-tape QTM by a single tape QTM is a central subject in this subsection.

We show that any multi-tape, well-formed QTM can be simulated by a certain well-formed, well-behaved QTM with concurrent head move. The simulation overhead here is a quadratic polynomial. This result makes it possible to simulate a multi-tape QTM by a single tape QTM with quadratic polynomial slowdown.

Proposition 1. Let M be a k-tape, well-formed QTM that halts in time $T(\mathbf{x})$ on input \mathbf{x} . There exists a (k+2)-tape, well-formed, well-behaved QTM M' with concurrent head move such that M', on input \mathbf{x} in tapes 1 to k and empty elsewhere, simulates M in time $2T(\mathbf{x})^2 + (2k+9)T(\mathbf{x}) + 4$. Moreover, if M is synchronous, dynamic, unidirectional, or normal form, so is M'. In particular, when M is synchronous, M' can be made stationary with extra $T(\mathbf{x}) + 1$ steps.

Proof. Given a QTM M, we construct a new QTM M' that simulates in 4r + 2k + 7 steps the rth step of M by moving its heads back and forth in all tapes concurrently and by expanding the simulation area by 2. Thus, the new QTM needs $\sum_{r=1}^{T(\boldsymbol{x})} (4r + 2k + 7)$ steps (with an additional pre-computation of 4 steps) to complete this simulation on input \boldsymbol{x} .

Let $M=(Q,\{q_0\},Q_f,\Sigma^k,\delta)$ be a given QTM. The desired M', starting from state \hat{q}_0 , works as follows. Initially, in four steps we mark \$ in the start cell in tape k+2 and we set up the simulation area of three cells (which are indexed -1,0,1) in tape k+1, each of which holds the record of the head position of M. We will maintain this record in tape k+1 by updating a symbol $(\sigma_i)_{1\leq i\leq k}$ in each cell, where $\sigma_i=1$ means that the ith tape head rests in the current cell. Finally, M' enters state $(q_0,\tau_0,\mathbf{d}_0)$, where $\boldsymbol{\tau}_0=\mathbf{d}_0=(\$)_{1\leq i\leq k}$.

At round $r, 1 \leq r \leq T(\boldsymbol{x})$, we simulate the rth step of the computation of M in 4r+2k+7 steps. We start with state $(p, \boldsymbol{\tau}_0, \boldsymbol{d}_0)$, provided that p is a current state of M. Moving the head rightward along all tapes toward the end of the simulation area, we collect the information on a k-tuple $\boldsymbol{\tau} = (\tau_i)_{1 \leq i \leq k}$ of tape symbols being scanned by M at time r and we then remember it by changing our internal state from $(p, \boldsymbol{\tau}_0, \boldsymbol{d}_0)$ to $(p, \boldsymbol{\tau}, \boldsymbol{d}_0)$. After the head arrives at the first blank cell, by applying the transition $\delta(p, \boldsymbol{\tau})$, we change $(p, \boldsymbol{\tau}, \boldsymbol{d}_0)$ into $(q, \boldsymbol{\tau}, \boldsymbol{d})$ if $\delta(p, \boldsymbol{\tau}, q, \boldsymbol{\sigma}, \boldsymbol{d})$ is non-zero. To end this simulation phase, we update the head position marked in tape k+1 (by using \boldsymbol{d}) and tape symbols (by using $\boldsymbol{\tau}$) by moving the head leftward to the first blank cell in tape k+1. Whenever the head reaches an end of the simulation area, we expand this area by 1 by writing the symbol $(0)_{1 \leq i \leq k}$ in its boundary blank cell. After the simulation phase, M' enters state $(q, \boldsymbol{\tau}_0, \boldsymbol{d}_0)$.

Suppose that M is in normal form. It is easy to verify that no well-formed QTM in normal form has more than two final state. Let q_f be a single final state of M. Adding the rule $\delta'((q_f, \boldsymbol{\tau}_0, \boldsymbol{d}_0), \boldsymbol{\sigma}) = |\hat{q}_0\rangle|\boldsymbol{\sigma}\rangle|\boldsymbol{R}\rangle$ makes M' be in normal form. If M' is synchronous, then M' can use the marker \boldsymbol{s} in tape k+2 to move its head back to the start cell and erase \boldsymbol{s} from the tape in $T(\boldsymbol{x})+1$ steps. This last movement forces M' to be stationary.

Any QTM with concurrent head move can reduce the number of tapes by merging a k-tuple of tape symbols which the head is scanning, into a single tape symbol.

Lemma 4. Let $1 \le m \le k$. Let M be a k-tape, well-formed QTM with concurrent head move that, on input \boldsymbol{x} in tapes 1 to m and empty elsewhere, halts in time $T(\boldsymbol{x})$. There exists an m-tape, well-formed QTM M' such that, on input \boldsymbol{x} , halts in time $T(\boldsymbol{x})$ and simulates the computation of M on \boldsymbol{x} . If M is dynamic, synchronous, stationary, unidirectional, or normal form, so is M'.

Simulation by Dynamic Machines. This subsection is devoted to show that any well-formed QTM can be simulated by a certain conservative QTM with quadratic polynomial slowdown.

Proposition 2. Let M be a k-tape, well-formed, synchronous QTM that halts in time $T(\mathbf{x})$ on input $\mathbf{x} \in \Sigma^k$. There exists a 2k-tape, well-formed, stationary, synchronous, unidirectional, dynamic QTM M' such that, on input \mathbf{x} in tape 1 to k and empty elsewhere, M' simulates M in time $2T(\mathbf{x})^2 + 16T(\mathbf{x}) + 4$. If M has a single final state, then M' is further in normal form.

Proof. The proof uses an idea of Yao [3]. Let $M = (Q, \{q_0\}, Q_f, \Sigma, \delta)$ be a given QTM with $Q_f = \{q_f^1, q_f^2, \dots, q_f^m\}$. We define the desired partial M' so that it simulates the r step of M by a round of 4r + 13 steps with all the heads moving concurrently. Since M requires $T(\boldsymbol{x})$ steps, M' needs $T(\boldsymbol{x}) \sum_{r=1}^{T(\boldsymbol{x})} (4r + 13)$ steps together with a pre- and post-computation of $T(\boldsymbol{x}) + 4$ steps, which gives the desired running time.

We first show the proposition for the special case k=1. Let $x=x_1x_2\cdots x_m$ be an input given in tape 1. In the initial phase, we create in four steps the configuration $(p_0, x_1'x_2\cdots x_m, -1, \$11, -1)$, where $x_1'=(q_0, x_1)$ and p_0 is a distinguished state of M' and symbol \$ is in the cell indexed -1.

To understand the simulation phase, we associate a configuration cf of M with a certain configuration cf' of M' defined in the following way. Assume that cf = (q, cont, k), where M in state q scans symbol σ in the cell indexed k and cont is the content of the tape. At the beginning of round r, $1 \le r \le T(\boldsymbol{x})$, we create the configuration cf' of M' which is of the form $(p_0, cont'_k, -r, 1^{r-1}\$1^{r+1}, -r)$, where $1^{r-1}\$1^{r+1}$ is written in tape 2 with \$ in the cell indexed -1 (which marks the simulation area) and $cont'_k$ is identical to cont except that the cell indexed k has symbol (q, σ) instead of σ .

To disregard any head direction that results from an application of δ , we treat as a single symbol the three consecutive symbols, where the head of M scans the middle symbol. In the course of the simulation, we first search in tape 2 the three consecutive symbols σ_0 ; (q, σ_1) ; σ_2 , where M in state q scans σ_1 , and encode them into the single symbol $(\sigma_0, (q, \sigma_1), \sigma_2)$ by moving the head back and forth. We then apply δ to this symbol with stepping right. This makes M' dynamic and also unidirectional. Finally, we decode the result and update the content of tape 2.

For each configuration at time r of M on input x, at the end of the simulation, M' produces its associated configuration. Therefore, when M enters a final configuration at time T(x), M' reaches a configuration in which a tape symbol of the form (q_f, σ) is found in tape 2. When M' finds such a symbol, it enters

its own final state \hat{q}_f in exactly $T(\boldsymbol{x})$ steps. Let δ_1' be the transition function for M'

For a general case $k \geq 1$, let $\boldsymbol{p} = (p_j)_{1 \leq j \leq k}$, $\boldsymbol{\sigma} = (\sigma_j)_{1 \leq j \leq k}$, and $\boldsymbol{\tau} = (\tau_j)_{1 \leq j \leq k}$. We first produce \S ; 1; 1 in tapes k+1 to 2k and enters state $\boldsymbol{p}_0 = (p_0)_{1 \leq j \leq k}$ with changing symbol σ_i in the start cell in tape i into (q_0, σ_i) . We then define $\delta'_k(\boldsymbol{p}, \boldsymbol{\sigma} * \boldsymbol{\tau})$ to be the product $\delta'_1(p_1, (\sigma_1, \tau_1)) \otimes \delta'_1(p_2, (\sigma_2, \tau_2)) \otimes \cdots \otimes \delta'_1(p_k, (\sigma_k, \tau_k))$. Clearly, this QTM is well-formed, stationary, and unidirectional. Note that the running time of the k-tape QTM M' does not depend on the number of tapes. Since M halts at time $T(\boldsymbol{x})$, M' finally enters state $(q_f^{i_j})_{1 \leq j \leq k}$ for some k-tuple $(i_j)_{1 \leq j \leq k}$ at time $2T(\boldsymbol{x})^2 + 16T(\boldsymbol{x}) + 4$.

In the case where M has a single final state q_f , we can add the new transition rule: $\delta'(\boldsymbol{q}_f, \boldsymbol{\sigma} * \boldsymbol{\tau}) = |\hat{q}_0\rangle|\boldsymbol{\sigma}, \boldsymbol{\tau}\rangle|\boldsymbol{R}\rangle$, where $\boldsymbol{q}_f = (q_f)_{1 \leq j \leq k}$, which makes M' be in normal form.

Since the proposition regards with a unidirectional QTM, it also gives an extension of Unidirection Lemma in [2] to multi-tape QTMs.

Simply combining Propositions 1 and 2 and Lemmas 3 and 4, we obtain the following corollary.

Corollary 1. Let M be a k-tape, well-formed QTM that, on input x in tape 1 and empty elsewhere, runs in time T(x). There exist a quartic polynomial and a two-tape conservative QTM M' such that, on input $(1^{T(x)}, x)$, M' halts in time p(T(x)) and satisfies $\mu_{M'}(1^{T(x)}, x) = \mu_M(x)$.

Note that, by modifying the simulation given in the proof of Proposition 1 (with $O(S(\boldsymbol{x})T(\boldsymbol{x}))$ slowdown, where $S(\boldsymbol{x})$ is any space bound of M), we can achieve a much tighter $O(T(x)^3)$ time bound. The detail is left to the reader.

Reversing a Computation. First recall Definition 4.11 in [2] that defines the notion: M_2 reverses the computation of M_1 . Different from [2], we only assume that M_1 and M_2 are well-formed QTMs (whose tape alphabets may differ) and that M_1 has a single final state. We show below that we can reverse the computation of any well-formed QTM with quadratic polynomial slowdown.

Theorem 1. Let M be a k-tape, well-formed QTM with a single final state that halts in time $T(\boldsymbol{x})$ on input \boldsymbol{x} . There exist a quadratic polynomial p and a 2(k+1)-tape, well-formed, synchronous, dynamic QTM M^R in normal form that, on input \boldsymbol{x} in tapes 1 to k and $1^{T(\boldsymbol{x})}$ in tape k+1 and empty elsewhere, reverses the computation of $\tilde{M}_{T,k+2}$ in time $p(T(\boldsymbol{x}))$.

Proof. Let $M = (Q, \{q_0\}, \{q_f\}, \Sigma^k, \delta)$ be a well-formed QTM. By Lemma 3, we have a (k+1)-tape, well-formed, synchronous QTM M_1 running in time $2T(\boldsymbol{x}) + 2$ on input $(\boldsymbol{x}, 1^{T(\boldsymbol{x})})$ that satisfies $M_1(|\boldsymbol{x}, 1^{T(\boldsymbol{x})}\rangle) = \tilde{M}_{T,1}(|\boldsymbol{x}, 1^{T(\boldsymbol{x})}\rangle)$.

By modifying the proof of Proposition 2, we can show the existence of a 2(k+1)-tape, well-formed, stationary, synchronous, unidirectional, dynamic QTM M_2 in normal form such that (i) M_2 on input $(\boldsymbol{x}, 1^{T(\boldsymbol{x})})$ halts in time $O(T(\boldsymbol{x})^2)$, (ii) when M_2 halts, tape k+1 consists only of its input $1^{T(\boldsymbol{x})}$ and tapes k+2 to

2k + 2 are empty, and (iii) $M_2(|\boldsymbol{x}, 1^{T(\boldsymbol{x})}\rangle)$ is identical to $M_1(|\boldsymbol{x}, 1^{T(\boldsymbol{x})}\rangle)$ when tapes k + 2 to 2k + 2 are ignored.

It is easy to extend Reversal Lemma in [2] to any multi-tape QTM. Let M^R be the QTM (as constructed in [2]) that reverses the computation of M_2 with extra two steps. Since M_2 is well-formed, synchronous, and dynamic, so becomes M^R because of its construction. Since any final superposition of M_2 is identical to that of $\tilde{M}_{T,k+2}$, the theorem follows.

Theorem 1 leads to the following lemma. The proof of the lemma also uses an argument similar to that of Theorem 4.14 in [1].

Lemma 5. (Squaring Lemma) Let $k \geq 2$. Let M be a k-tape, well-formed QTM with a single final state which, on input \mathbf{x} , outputs $b(\mathbf{x}) \in \{0,1\}$ in the start cell of tape k in time $T(\mathbf{x})$ with probability $\rho(\mathbf{x})$. There exist a quadratic polynomial p and a (2k+3)-tape, well-formed, stationary, normal form QTM M' such that, on input $(1^{T(\mathbf{x})}, \mathbf{x})$, M' reaches in time $p(T(\mathbf{x}))$ the configuration in which M' is in a single final state with $1^{T(\mathbf{x})}$ in tape 1, \mathbf{x} in tapes 2 to k, $b(\mathbf{x})$ in tape k+1, and empty elsewhere, with probability $\rho(\mathbf{x})^2$.

Proof. Let M be a given QTM. By Theorem 1, there exists a 2(k+1)-tape, well-formed, synchronous, dynamic, normal form QTM M^R that, on input $(1^{T(\boldsymbol{x})}, \boldsymbol{x})$, reverses the computation of $\tilde{M}_{T,k+2}$ in time $O(T(\boldsymbol{x})^2)$.

We define the desired QTM M' as follows. Let $(1^{T(\boldsymbol{x})}, \boldsymbol{x})$ be any input. Starting with its initial configuration cf_0 , M' runs $\tilde{M}_{T,k+2}$ with ignoring tape 2k+3. Consider the final superposition $\tilde{M}_{T,k+2}(|1^{T(\boldsymbol{x})},\boldsymbol{x}\rangle)$. When $\tilde{M}_{T,k+2}$ halts, M' copies the content of the start cell in the output tape into tape 2k+3 in two extra steps. Now we have the superposition $|\phi\rangle = \sum_y \alpha_{\boldsymbol{x},y}|y\rangle|b_y\rangle$, where $b_y \in \{0,1\}$ is the content of tape 2k+3 and y ranges over all configurations excluding the status of tape 2k+3. Next, M' runs M^R starting with $|\phi\rangle$ with ignoring tape 2k+3. Note that $M^R(|\phi'\rangle) = |cf_0\rangle|b(\boldsymbol{x})\rangle$ for the superposition $|\phi'\rangle = \sum_y \alpha_{\boldsymbol{x},y}|y\rangle|b(\boldsymbol{x})\rangle$.

By a simple calculation, we have $\langle \phi' | \phi \rangle = \sum_{y:b_y=b(\boldsymbol{x})} |\alpha_{\boldsymbol{x},y}|^2$, which equals $\rho(\boldsymbol{x})$ since $\tilde{M}_{T,2k+3}$ outputs $b(\boldsymbol{x})$ with probability $\rho(\boldsymbol{x})$.

Since M^R preserves the inner product, $\langle M^R(|\phi'\rangle)|M^R(|\phi\rangle)\rangle = \langle \phi'|\phi\rangle$, which is the amplitude in $M'(|1^{T(\boldsymbol{x})}, \boldsymbol{x}\rangle)$ of $|cf_0\rangle|b(\boldsymbol{x})\rangle$. Thus, the squared magnitude of amplitude of $|cf_0\rangle|b(\boldsymbol{x})\rangle$ is exactly $\rho(\boldsymbol{x})^2$.

Timing Problem. Let $M = (Q, \{q_0\}, \{q_f\}, \Sigma^k, \delta)$ be a k-tape, partial, well-formed, normal form QTM. We assume that any computation path of M on input \boldsymbol{x} is completely determined by δ and ends with final state q_f and that the length of any computation path of M on x does not exceed $T(\boldsymbol{x})$. We modify δ by forcing $\delta(q_f, \boldsymbol{\sigma})$ to be $|q_f\rangle|\boldsymbol{\sigma}\rangle|\boldsymbol{N}\rangle$ for any $\boldsymbol{\sigma}\in \Sigma^k$ and let δ_* denote this modified δ . This δ_* makes M halt within time $T(\boldsymbol{x})$. For clarity, let M_* be the QTM defined by δ_* . Although M_* may not be well-formed, when the final superposition has unit L_2 -norm, we can still consider the acceptance probability of M_* as before. Can we simulate M_* on a well-formed QTM?

For convenience, we say that M is well-structured if (1) it is well-formed, (2) any computation path of M on input x is completely determined by δ and ends with a single final state, and (3) any final superposition of M_* on each input has unit L_2 -norm. For simplicity, we write $\mu_M(x)$ to denote the acceptance probability of M_* on input x.

Lemma 6. Let M be a k-tape, well-structured, partial QTM in normal form such that the length of any computation path of M on each input \boldsymbol{x} is less than $T(\boldsymbol{x})$. There exists a (k+3)-tape, well-formed QTM M' such that, on input \boldsymbol{x} in tapes 1 to k and $1^{T(\boldsymbol{x})}$ in tape k+1 and empty elsewhere, it halts in time $O(T(\boldsymbol{x})^2)$ and satisfies $\mu_{M'}(\boldsymbol{x}, 1^{T(\boldsymbol{x})}) = 2^{-\lfloor \log T(\boldsymbol{x}) \rfloor - 1} \mu_M(\boldsymbol{x})$.

Proof. Let M be a given QTM. We first construct a well-formed QTM M_1 running in time $O(T(\boldsymbol{x})^2)$ on input $(\boldsymbol{x}, 1^{T(\boldsymbol{x})})$ such that the probability that M halts in an accepting configuration in which tape k+2 consists only of symbols $0^{\lfloor \log T(\boldsymbol{x}) \rfloor + 2}$, is $2^{-\lfloor \log T(\boldsymbol{x}) \rfloor - 1} \mu_M(\boldsymbol{x})$.

- 1. We produce in tape k+3 the "reversed" binary representation of T(x) in exactly $2T(x)^2 + 12T(x) + 9$ steps. Using this representation, we produce $|\log T(x)| + 1$ bit zeros (following control bit 1) in tape k+2.
- 2. We simulate M's move by incrementing two counters. The first counter is in tape k+1, of unary form, and the second one is a binary counter in tape k+2. At each round of simulating a single step of M, M_1 also increments the unary counter by stepping right and increments the binary one (using control bit 1) in exactly $2\lfloor \log T(\boldsymbol{x}) \rfloor + 8$ steps. When M terminates, M_1 keeps incrementing the unary counter but idles on the binary counter for each $2\lfloor \log T(\boldsymbol{x}) \rfloor + 8$ steps (using control bit 0 in tape k+2 for reversibility).
- 3. After $T(\boldsymbol{x})$ rounds, we apply a Hadamard transform, with stepping right, to the content of the binary counter except its control bit (i.e., $\delta'(p, \boldsymbol{\sigma} * \sigma') = \frac{1}{\sqrt{2}} \sum_{\tau \in \{0,1\}} (-1)^{\sigma' \cdot \tau} |p\rangle |\boldsymbol{\sigma}, \tau\rangle |\boldsymbol{N}, R\rangle$, where σ' is in tape k+2). Since the length of this counter is $\lfloor \log T(\boldsymbol{x}) \rfloor + 1$, we can observe symbols $0 \circ 0^{\lfloor \log T(\boldsymbol{x}) \rfloor + 1}$ in tape k+2 with amplitude $2^{-\lfloor \log T(\boldsymbol{x}) \rfloor 1}$. Hence, the probability that M reaches an accepting configuration with $0^{\lfloor \log T(\boldsymbol{x}) \rfloor + 2}$ in tape k+2 is $2^{-\lfloor \log T(\boldsymbol{x}) \rfloor 1} \mu_M(\boldsymbol{x})$.

We design M' so that the heads in tapes k+1 to k+3 return to the start cells (using $1^{T(\boldsymbol{x})}$ in tape k+1) and the rest of heads stay in the same cells as M's. It is easy to see that M_1 is in normal form if we add the rule: $\delta'(q_f, \boldsymbol{\sigma}) = |q_0\rangle|\boldsymbol{\sigma}\rangle|\boldsymbol{N}\rangle$. Moreover, if M is stationary, M_1 is also stationary.

For the desired machine M', we design it to accept input $(\boldsymbol{x}, 1^{T(\boldsymbol{x})})$ exactly when M_1 reaches an accepting configuration with $0^{\lfloor \log T(\boldsymbol{x}) \rfloor + 2}$ written in tape k+2. It thus follows that $\mu_{M'}(\boldsymbol{x}, 1^{T(\boldsymbol{x})}) = 2^{-\lfloor \log T(\boldsymbol{x}) \rfloor - 1} \mu_M(\boldsymbol{x})$.

Lemma 6 solves the timing problem for any quantum complexity class whose acceptance criteria is invariant to a polynomial fraction of acceptance probability.

5 Oracle Quantum Turing Machines

Unlike the previous sections, we will focus on an oracle QTM, which is a natural extension of a classical oracle TM with the help of a set of oracles.

Formally, we define a (k+m)-tape oracle QTM M with m query tapes to be a septuple $(Q, \{q_0\}, Q_f, Q_p, Q_a, \Sigma_1 \times \Sigma_2 \times \cdots \times \Sigma_{k+m}, \delta)$, where Q includes $Q_p = \{q_p^1, q_p^2, \dots, q_p^m\}$, a set of pre-query states, and $Q_a = \{q_a^1, q_a^2, \dots, q_a^m\}$, a set of post-query states, and the transition function δ is defined only on $(Q - Q_p) \times \Sigma^k$. We assume the reader's familiarity with an oracle query. For its definition, see [2]. Conventionally, we assume that every alphabet Σ_{k+i} , $1 \leq i \leq m$, includes binary bits $\{0,1\}$. Let $\mathcal{A} = (A_i)_{1 \leq i \leq m}$ be a series of oracles such that each A_i is a subset of $(\Sigma_{k+i})^*$. Note that query states q_p^i and q_a^i correspond only to the ith query tape and the ith oracle A_i .

It is important to note that Well-Formedness Lemma and Completion Lemma hold even for oracle QTMs.

Reducing the Number of Query Tapes. We can reduce the number of query tapes by combining a given set of oracles into a single oracle together with copying a query word written in one of query tapes into a single query tape. When we copy a query word $y \circ b$ from the *i*th query tape, we pad the suffix $0^{i}1^{m-i}$ (between y and b) to make the copying process reversible.

Lemma 7. Let $m \geq 2$. Let M be a (k+m)-tape, well-formed, oracle QTM with m query tapes that halts in time $T(\boldsymbol{x})$ on input $\boldsymbol{x} \in \Sigma^k$. Let $\mathcal{A} = (A_i)_{1 \leq i \leq m}$ be a series of oracles. There exists a (k+2m+1)-tape, well-formed, oracle QTM M' with a single query tape such that, on input $(\boldsymbol{x}, 1^{T(\boldsymbol{x})})$, halts in time $5T(\boldsymbol{x})^2 + 8T(\boldsymbol{x})$ and $\mu_{M'}^B(\boldsymbol{x}, 1^{T(\boldsymbol{x})}) = \mu_M^A(\boldsymbol{x})$, where $B = \{y0^i1^{m-i} \mid y \in A_i\}$.

Adjusting the Number of Queries. Let M be a given QTM. At the end of each round, in which a new QTM M' simulates a single step of the computation of M, we force M' to make a query (of the form $0 \circ 0$) in 6 steps if M does not query. When M invokes an oracle query, we force M' to idle for 6 steps instead of making a query of $0 \circ 0$. This proves the lemma below.

Lemma 8. Let M be a (k+1)-tape, well-formed, oracle QTM in normal form with a single query tape that halts in time $T(\mathbf{x})d$, on input $\mathbf{x} \in \Sigma^k$. Let A be an oracle. There exist a (k+2)-tape, well-formed, oracle QTM M' with two query tapes running in time $TT(\mathbf{x})$ on input \mathbf{x} such that M' makes exactly $T(\mathbf{x})$ queries along each computation path and $\mu_{M'}^{(A,A)}(\mathbf{x}) = \mu_M^A(\mathbf{x})$.

Adjusting the Length of Query Words. We show that the length of query words can be stretched with quadratic slowdown. To extend the length of a query word to the fixed length T-1, we pad the suffix $01^{T-|y|-2}$ in 4T+6 steps.

Lemma 9. Let M be a (k+1)-tape, well-formed, oracle QTM in normal form with a single query tape that halts in time $T(\mathbf{x})$ on input $\mathbf{x} \in \Sigma^k$. Let A be an oracle set. There exists a (k+3)-tape, well-formed, oracle QTM M' such that, for every input $(\mathbf{x}, 1^{T(\mathbf{x})})$, it halts in time $4T(\mathbf{x})^2 + 10T(\mathbf{x})$, the length of any query word is exactly $T(\mathbf{x}) - 1$ on any computation path, and it satisfies $\mu_{M'}^B(\mathbf{x}, 1^{T(\mathbf{x})}) = \mu_M^A(\mathbf{x})$, where $B = \{y01^{m-|y|-2} \mid y \in A, m \geq |y|+2\}$.

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