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#### Abstract

Distributed quantum systems and especially the Quantum Internet have the ever-increasing potential to fully demonstrate the power of quantum computation. This is particularly true given that developing a general-purpose quantum computer is much more difficult than connecting many small quantum devices. One major challenge of implementing distributed quantum systems is programming them and verifying their correctness. In this paper, we propose a CSP-like distributed programming language to facilitate the specification and verification of such systems. After presenting its operational and denotational semantics, we develop a Hoare-style logic for distributed quantum programs and establish its soundness and (relative) completeness with respect to both partial and total correctness. The effectiveness of the logic is demonstrated by its applications in verification of quantum teleportation and local implementation of non-local CNOT gates, two important algorithms widely used in distributed quantum systems.

#### 1 Introduction

Quantum computers exploit quantum phenomena such as superposition and entanglement to perform computation. The past five years have seen exciting progresses in building small-scale quantum processors and the two state-of-the-arts, Google's Sycamore and IBM Q Rochester, both have 53 qubits. While these small quantum devices already demonstrate certain advantages over classical supercomputers, large scale general-purpose quantum computers are still far from reach.

The Quantum Internet has been proposed as a key strategy to provide large-scale quantum computing [25, 37, 26, 10]. The idea is to connect many small quantum devices by using quantum communications and this network of quantum devices will then have the functionality of a (virtual) large-scale quantum computer. On July 3, 2020, the Department of Energy of the United States proposed a 10-year roadmap for a national Quantum Internet under the \$1.2 billion National Quantum *Initiative Act.* Several important steps have been experimented in the past two years. In February 2020, scientists from Argonne and the University of Chicago successfully entangled photons across a 52-mile underground network of optical fibre. In April 2021, a team of researchers from QuTech in the Netherlands reported realisation of the first entanglement-based quantum network (connecting three quantum processors) [30].

As pointed out in [26], software-defined networking (SDN) technology is particularly important for quantum networks, because under current technical conditions, quantum memories have a very short lifespan. On the other hand, programming quantum networks is much harder and more errorprone than programming classical ones due to the possible existence of entanglement between different systems and non-commutativity of quantum observables and operations.

Inspired by Apt's work [2] on distributed programming based upon Hoare's CSP (Concurrent Sequential Processes) [21], we define in this paper a programming language for distributed quantum systems. Recall that a distributed system consists of a number of spatially separated processes that work independently using their private storage, but communicate by explicit message passing.

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Our language supports both classical and quantum operations of individual processes. However, to make the presentation simpler, we only consider classical communication between different processes. Note that this is not a serious limitation, as generic quantum communication can be achieved by using the teleportation protocol [5] provided that entanglement is pre-shared between relevant parties. Furthermore, communication is achieved in a handshaking (or rendezvous) way; that is, the sender can deliver a message only when the receiver is ready to accept it at the same moment. We leave the asynchronous communication of quantum states as future work. Based on the notion of classical-quantum assertions defined in [16], we propose Hoare-style logic systems for both partial and total correctness of distributed quantum programs, and prove their soundness and (relative) completeness. The effectiveness of these logic systems are demonstrated through the verification of quantum teleportation and local implementation of non-local CNOT gates, two important algorithms widely used in distributed quantum systems. It is worth noting that since the language we consider includes probabilistic assignments, this paper actually provides a sound and relatively complete Hoare logic for distributed probabilistic programs as a by-product.

Technical Contributions: While the semantics and proof systems in this paper are defined in a way similar to that of [16], the extension from sequential quantum programs to distributed quantum programs is challenging.

Firstly, the operational semantics of quantum measurements and probabilistic assignments in [16] are given in a 'nondeterministic' way, with the probabilities of different branches being encoded in the quantum part of the configurations. This follows a tradition originated in [32] and adopted in [39, 40] that simplifies both notationally and conceptually the semantics of (deterministic) quantum languages, especially the description of non-termination. However, distributed quantum programs investigated in this paper exhibit real nondeterminism (in the transition systems for operational semantics) due to the possible interleaving of local actions and communication of different sequential processes. To distinguish these two types of nondeterminism, we model quantum measurements and probabilistic assignments in a (standard) probabilistic way. Accordingly, the transition relation between configurations has to be lifted to probability distributions of configurations.

Secondly, despite that the entire distributed program may exhibit nondeterminism even if each individual process is deterministic, we show that different computations from a given configuration actually obtain the same classical-quantum state, thanks to the disjointness of the (classical changeable and quantum) variables accessible by different processes. This result clears the obstacle in defining the denotational semantics of distributed quantum programs and ensures that a distributed program can be sequentialised into a deterministic one without affecting its semantics.

Thirdly, the proof systems presented in [16] are designed for sequential quantum programs. New techniques are developed in this paper in extending them to distributed programs and proving their soundness and relative completeness.

Organisation of the paper: In the rest of this section, we briefly discuss some related works and present quantum teleportation as a motivating example. The remainder of this paper is organised as follows. In Sec. 2, we present the three layers of the syntax of the distributed quantum programming language, which is followed by its operational and denotational semantics in Sec. 3. In particular, we prove that distributed quantum programs are semantically deterministic in the sense that different computations from a given configuration always give the same classical-quantum state. We then show in Sec. 4 how a distributed quantum program can be sequentialised without affecting its semantics. Based on the notion of classical-quantum assertion, we present a Hoare-style logic in Sec. 5 for distributed quantum programs and establish its soundness and (relative) completeness for both partial and total correctness. The last section concludes this paper with an outline of future works. Due to space limitation, we omit all proofs as well as the verification of quantum teleportation and local implementation of non-local CNOT gates. Interested readers may find these details in the appendix.

### 1.1 Related Works

The following three lines of previous works are closely related to this paper.

**Quantum Process Algebras**: Process algebra is the mainstream approach to formally model and reason about quantum communication systems. Since 2004, several quantum process algebras such as QPAlg [23], CQP [17], and qCCS [13, 42, 15] have been introduced and adopted in verification of popular quantum communication protocols such as teleportation [5] and superdense coding [6]. Following [2] (also see [1], Chapter 11), we choose to use (a subset of) a quantum extension of process algebra CSP as our language for programming distributed quantum systems, but use a Hoare-style logic to reason about their correctness.

**Quantum Hoare Logic**: Hoare logic provides a syntax-oriented proof system to reason about program correctness [20]. In recent years, Hoare-style logics for quantum programs have been developed in [9, 14, 24, 39, 35, 16]. However, these logic systems are designed for the verification of sequential quantum programs, thus are not suitable for the distributed ones considered in the current paper. Nevertheless, our definition of semantics of distributed quantum programs is based on the key notions such as classical-quantum states and assertions introduced in [16].

**Programming with Quantum Communication**: The authors of [33] presented some interesting ideas of specifying and analysing quantum communication in a predicative programming language. However, the key technique for verification of quantum communication protocols developed in [33] (and in predicative programming [19] in general) is refinement, while we use a Hoare-style logic here.

# 1.2 Motivating Example — Quantum Teleportation

Quantum teleportation was proposed by Bennett et al. [5] for transmitting *quantum information* (e.g. the exact state of an atom or photon) via only *classical communication* but with the help of previously shared *quantum entanglement* between the sender and the receiver. It is one of the most surprising examples where entanglement helps to accomplish a certain task that is impossible in the classical world. A large number of quantum communication protocols such as quantum gate teleportation [18], port-based teleportation [22], quantum repeaters [7], and measurement based quantum computing [31] have been designed based on it, and some of them have been experimentally implemented [29].

Let us consider the simplest case of teleporting a qubit. Assume that Alice and Bob live far apart and there is only a classical communication channel between them. But Alice wants to send quantum information, say a state  $|\psi\rangle \triangleq \alpha_0 |0\rangle + \alpha_1 |1\rangle$  of qubit q, to Bob. How can she do it? This seems a task impossible for her to accomplish because it may take infinite amount of classical information to describe the complex amplitudes  $\alpha_0$  and  $\alpha_1$ . However, if Alice and Bob share entanglement; more precisely, if they possess qubits  $q_1$  and  $q_2$  respectively and these two qubits are in the Bell state  $|\beta\rangle \triangleq \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$  (also called EPR pair), then they can accomplish the task using the following protocol, called *teleportation*:

- (1) Alice interacts qubit q in state  $|\psi\rangle$  and her half  $q_1$  of the shared EPR pair  $|\beta\rangle$  by performing first the controlled NOT (CNOT for short) on  $q, q_1$  and then the Hadamard gate H on q, where:
  - = the CNOT acts as follows: if the control qubit q is in  $|0\rangle$  then the target qubit  $q_1$  is left unchanged, and if q is in  $|1\rangle$  then  $q_1$  is flipped between  $|0\rangle$  and  $|1\rangle$ ;
  - = the *H* gate turns basis states  $|0\rangle$  and  $|1\rangle$  to their equal superposition  $|+\rangle$  and  $|-\rangle$ , where  $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$ , respectively.
- (2) Alice measures her qubits  $q, q_1$  (in the standard basis), and sends the obtained results classical bits z, x through the classical channel to Bob.
- (3) On his half q₂ of the EPR pair, Bob performs operation X whenever the received classical information x = 1, and then Z whenever z = 1. Here X and Z are Pauli operations with X|i⟩ = |1 i⟩ and Z|i⟩ = (-1)<sup>i</sup>|i⟩ for i = 0, 1.



**Figure 1** Quantum Teleportation. The wires from top to bottom represent qubits q,  $q_1$ , and  $q_2$  respectively. Furthermore, q and  $q_1$  belong to Alice while  $q_2$  belongs to Bob.

Quantum teleportation can be visualised as the quantum circuit in Figure 1. What surprises us is that at the end Bob's qubit  $q_2$  is in state  $|\psi\rangle$ . In other words, Alice sends the quantum information  $|\psi\rangle$  to Bob only by classical communication of two bits in step (2), even without knowing the amplitudes  $\alpha_0$  and  $\alpha_1$  of  $|\psi\rangle$ . Of course, this is achieved by consuming some entanglement (At the end of the protocol, qubits  $q_1$  and  $q_2$  are no longer entangled).

# 2 A Language for Programming Distributed Quantum Systems

We propose a programming language to describe distributed quantum systems. The syntax has three layers, introduced in the following three subsections respectively.

# 2.1 Sequential quantum programs

For the first layer, we extend the classical-quantum while language defined in [16] with alternative and repetitive commands [11]. We assume two basic types for classical variables: **Boolean** with the corresponding domain  $D_{\text{Boolean}} \triangleq \{\text{true, false}\}$  and Integer with  $D_{\text{Integer}} \triangleq \mathbb{Z}$ . For each integer  $d \ge 1$ , we assume a basic quantum type **Qudit** with domain  $\mathcal{H}_{\text{Qudit}}$ , which is a *d*-dimensional Hilbert space with an orthonormal basis  $\{|0\rangle, \ldots, |d-1\rangle\}$ . In particular, we denote the quantum type for d = 2 as **Qubit**. Let cVar, ranged over by  $x, y, \cdots$ , and qVar, ranged over by  $q, r, \cdots$ , be countably infinite sets of classical and quantum variables, respectively. Denote by type(v)the type of a (classical or quantum) variable v. For any finite subset V of qVar, let  $\mathcal{H}_V \triangleq \bigotimes_{q \in V} \mathcal{H}_q$ , where  $\mathcal{H}_q \triangleq \mathcal{H}_{type(q)}$ . In this paper, when we refer to a subset of qVar, it is always assumed to be finite.

With the above notions, a sequential quantum program is defined by the following syntactic rules:

$$S ::= \mathbf{skip} \mid \mathbf{abort} \mid x := e \mid x :=_{\$} g \mid x := \mathbf{meas} \ \mathcal{M}[\bar{q}] \mid q := 0 \mid \bar{q} := U \mid S_0; S_1$$
  
$$\mathbf{if} \ B_1 \to S_1 \square \dots \square B_n \to S_n \ \mathbf{fi} \mid \mathbf{do} \ B_1 \to S_1 \square \dots \square B_n \to S_n \ \mathbf{od}$$

where S and  $S_i$  are sequential quantum programs, x a classical variable in cVar, e a classical expression with the same type as x, g a discrete probability distribution over  $D_{type(x)}$ ,  $B_i$  a **Boolean**-type expression, q a quantum variable and  $\bar{q} \triangleq q_1, \ldots, q_n$  a (ordered) tuple of distinct quantum variables in qVar,  $\mathcal{M}$  a measurement and U a unitary operator on  $d_{\bar{q}}$ -dimensional Hilbert space with

$$d_{\bar{q}} \triangleq \dim(\mathcal{H}_{\bar{q}}) = \prod_{i=1}^{n} \dim(\mathcal{H}_{q_i}).$$

Sometimes we also use  $\bar{q}$  to denote the (unordered) set  $\{q_1, q_2, \ldots, q_n\}$ . Let  $|\bar{q}| \triangleq n$  be the size of  $\bar{q}$ . We write  $x := \text{meas } \bar{q}$  for  $x := \text{meas } \mathcal{M}_{com}[\bar{q}]$  where  $\mathcal{M}_{com} \triangleq \{P_k \triangleq |k\rangle \langle k| : 0 \leq k < d_{\bar{q}}\}$  is the projective measurement according to the computational basis of  $\mathcal{H}_{\bar{q}}$ . We always write  $|k\rangle$  for the product state  $|k_1\rangle \cdots |k_n\rangle$ , where  $k = \sum_{i=1}^n k_i d_{q_{i+1}} \cdots d_{q_n}$ .

The alternative and repetitive commands above are sometimes abbreviated as

if  $\Box_{i=1}^n B_i \to S_i$  fi and do  $\Box_{i=1}^n B_i \to S_i$  od

respectively. For simplicity, we only consider deterministic sequential quantum programs in this paper. To this end, we assume that the  $B_i$ 's are mutually exclusive; that is, for each  $i, B_i \to \bigwedge_{j \neq i} \neg B_j$  is a tautology. However, we do not require  $\bigvee_{i=1}^n B_i \leftrightarrow \text{true}$ . Under this assumption, a guarded command  $B_i \to S_i$  in if  $\Box_{i=1}^n B_i \to S_i$  fi will be chosen to execute once its guard  $B_i$  evaluates to true. If all guards evaluate to false, the alternative command will lead to a (classical) *failure* state, which is a feature introduced in [11] but does not exist in the while language of [16]. The selection of guarded commands in do  $\Box_{i=1}^n B_i \to S_i$  od follows a similar way, with the only difference that after termination of a selected  $S_i$  the whole command is repeated. Moreover, in contrast with the alternative command, the repetitive command properly terminates if all the guards evaluate to false.

# 2.2 Sequential quantum process

To describe the second syntactic layer for distributed quantum programs, we adopt a subset of Hoare's CSP (Communicating Sequential Processes) [21, 8], following the approach in [1]. Let *chan* be a set of (classical) channel names, ranged over by  $c, d, \ldots$ . An *input command* is of the form c?x, while an *output command* is of the form c!e, where  $c \in chan$  is a communication channel,  $x \in cVar$  a classical variable, and e an expression. Intuitively, c?x expresses the request to receive a classical value along channel c. Upon reception this value is assigned to variable x. In contrast, c!e expresses the request to send the value of expression e along channel c. A *generalised guard* is of the form  $g \triangleq B$ ;  $\alpha$  where B is a Boolean expression, and  $\alpha$  an input or output command. In particular, if  $B \equiv \mathbf{true}$ , then we denote g simply as  $\alpha$ .

Let  $\alpha_1$  and  $\alpha_2$  be two input/output (i/o) commands. They are said to *match* if they refer to the same channel, one of them is an input, and the other one output with the same type. Given two matched i/o commands  $\alpha_1 \triangleq c?x$  and  $\alpha_2 \triangleq c!e$ , the *communication effect* of  $\alpha_1$  and  $\alpha_2$  is defined to be the program statement x := e; that is,

$$Effect(\alpha_1, \alpha_2) = Effect(\alpha_2, \alpha_1) \triangleq x := e.$$

▶ **Definition 1.** A sequential quantum process has the form:

$$S ::= S_0;$$
 do  $\Box_{i=1}^m B_i; \alpha_i \to S_i$  od

where  $m \ge 0, S_0, S_1, \ldots, S_m$  are sequential quantum programs defined in the previous subsection. Again, we assume that  $B_j$ 's are mutually exclusive. We call  $S_0$  the *initialisation part*, and do  $\Box_{j=1}^m B_j; \alpha_j \to S_j$  od the *main loop* of S. If m = 0, then we let  $S = S_0$ . In this way, any sequential quantum program is a sequential process. If  $S_0 \equiv \mathbf{skip}$ , we drop  $S_0$  from S unless m = 0.

We have the following notations for sequential quantum process S.

- Denote by cv(S) and qv(S) the sets of classical and quantum variables appearing in S, respectively. Note that we do not distinguish between free and bound variables; that is, the classical variable appearing in an input command of S is also included in cv(S). Let  $var(S) \triangleq cv(S) \cup qv(S)$ .
- Denote by change(S) the set of classical variables that appear on the left-hand side of an assignment or in an input command in S. Note that the only way to retrieve information from a quantum system is to measure it, which may change its state. Thus qv(S) is also the set of changeable quantum variables in S.
- Denote by chan(S) the set of channel names appearing in S.

# 2.3 Distributed quantum programs

Now we are ready to define the syntax for distributed quantum programs.

▶ Definition 2. A distributed quantum program is a parallel composition S ::= S<sub>1</sub> || ··· ||S<sub>n</sub> where n ≥ 1 and S<sub>1</sub>,..., S<sub>n</sub> are sequential quantum processes defined in the above subsection which satisfy
Pairwise disjointness: for all 1 ≤ i ≠ j ≤ n, var(S<sub>i</sub>) ∩ (change(S<sub>j</sub>) ∪ qv(S<sub>j</sub>)) = Ø;
Point-to-point connection: for all 1 ≤ i < j < k ≤ n, chan(S<sub>i</sub>) ∩ chan(S<sub>j</sub>) ∩ chan(S<sub>k</sub>) = Ø. Let cv(S) ≜ ⋃<sub>i=1</sub><sup>n</sup> cv(S<sub>i</sub>), and change(S), qv(S), and var(S) be similarly defined.

Essentially, the first clause requires that (1) classical variables in any process cannot be changed by other processes; (2) quantum variables in any process do not appear in other processes. The second clause in Definition 2 implies that each communication channel is shared by at most two processes. This constraint, together with the assumption that sequential processes are deterministic, means that at any moment, each process is only able to communicate with at most one other process. Note also that we disallow nested parallelism in distributed programs. Finally, any sequential quantum process is a distributed quantum program with n = 1.

The constraints in Definition 2 look very strict at the first glance. However, using similar approaches presented in [3, 43], more general distributed quantum systems can be transformed into this special form by introducing control variables (say,  $stage_A$  and  $stage_B$  in the following example).

► **Example 3** (Quantum Teleportation as a Distributed Program). The quantum teleportation protocol presented in Sec. 1.2 can be written as a distributed program *Teleport*  $\triangleq$  *Alice*  $\parallel$  *Bob* where *Alice*  $\triangleq$ 

$$q, q_1 := CNOT; q := H; z_A := meas q; x_A := meas q_1; stage_A := 0;$$
  
 $\mathbf{do} \ stage_A = 0; c!x_A \to stage_A := 1 \square \ stage_A = 1; d!z_A \to stage_A := 2 \ \mathbf{od}$ 

and  $Bob \triangleq$ 

 $stage_B := 0;$  **do**  $stage_B = 0; c?x_B \rightarrow stage_B := 1;$  **if**  $x_B = 1 \rightarrow q_2 *= X \Box \neg (x_B = 1) \rightarrow skip$  **fi**   $\Box stage_B = 1; d?z_B \rightarrow stage_B := 2;$  **if**  $z_B = 1 \rightarrow q_2 *= Z \Box \neg (z_B = 1) \rightarrow skip$  **fi od** 

# 3 Operational and Denotational Semantics

We recall some basic notions from [16] to define the semantics of distributed quantum programs.

#### 3.1 Classical-quantum states

Let  $\Sigma \triangleq c Var \to D$  be the (uncountably infinite) set of *classical states*, where  $D \triangleq D_{\text{Boolean}} \cup D_{\text{Integer}}$ . We further require that states in  $\Sigma$  respect the types of classical variables; that is,  $\sigma(x) \in D_{type(x)}$  for all  $\sigma \in \Sigma$  and  $x \in cVar$ . For  $V \subseteq qVar$ , let  $\mathcal{D}(\mathcal{H}_V)$  be the set of partial density operators on  $\mathcal{H}_V$ ; that is, positive linear operators with the trace being less than or equal to 1. Furthermore, let  $\mathbf{0}_{\mathcal{H}_V} \in \mathcal{D}(\mathcal{H}_V)$  be the zero operator on  $\mathcal{H}_V$ .

▶ **Definition 4.** Given  $V \subseteq qVar$ , a *classical-quantum state* (cq-state for short)  $\Delta$  on V is a function in  $\Sigma \rightarrow \mathcal{D}(\mathcal{H}_V)$  such that

the support of Δ, denoted [Δ], is countable. That is, Δ(σ) ≠ 0<sub>H<sub>V</sub></sub> for at most countably infinite many σ ∈ Σ;

 $\langle \mathbf{skip}, \sigma, \rho \rangle \rightarrow \langle E, \sigma, \rho \rangle$  $\langle x := e, \sigma, \rho \rangle \rightarrow \langle E, \sigma[\sigma(e)/x], \rho \rangle$  $\langle q := 0, \sigma, \rho \rangle \to \langle E, \sigma, \sum_{i=0}^{d_q-1} |0\rangle_q \langle i|\rho|i\rangle_q \langle 0| \rangle$  $\langle \bar{q} *= U, \sigma, \rho \rangle \rightarrow \langle E, \sigma, U_{\bar{q}} \rho U_{\bar{q}}^{\dagger} \rangle$  $\frac{\mathcal{M} = \{M_i : i \in I\}, \ \rho_i = M_i \rho M_i^{\dagger}, \ p_i = \operatorname{tr}(\rho_i)}{\langle x := \operatorname{\mathbf{meas}} \mathcal{M}[\bar{q}], \sigma, \rho \rangle \to \sum_{p_i > 0} p_i \cdot \langle E, \sigma[i/x], \rho_i/p_i \rangle}$  $\overline{\langle x :=_{\$} g, \sigma, \rho \rangle} \to \sum_{d \in D_{tupe(x)}} g(d) \cdot \langle E, \sigma[d/x], \rho \rangle$  $\sigma \models B_i, 1 \le i \le n$  $\sigma \models \bigwedge_{i=1}^n \neg B_i$  $\overline{\langle \mathbf{if} \square_{i=1}^{n} B_i \to S_i \, \mathbf{fi}, \sigma, \rho \rangle \to \langle E, \mathbf{fail}, \rho \rangle}$  $\overline{\langle \mathbf{if} \square_{i=1}^{n} B_i \to S_i \mathbf{fi}, \sigma, \rho \rangle \to \langle S_i, \sigma, \rho \rangle}$  $\frac{\sigma \models \bigwedge_{i=1}^{n} \neg B_{i}}{\langle \mathbf{do} \, \Box_{i=1}^{n} B_{i} \rightarrow S_{i} \, \mathbf{od}, \sigma, \rho \rangle \rightarrow \langle E, \sigma, \rho \rangle}$  $\sigma \models B_i, 1 \le i \le n$  $\overline{\langle \operatorname{\mathbf{do}} \square_{i=1}^{n} B_{i} \to S_{i} \operatorname{\mathbf{od}}, \sigma, \rho \rangle} \to \overline{\langle S_{i}; \operatorname{\mathbf{do}} \square_{i=1}^{n} B_{i} \to S_{i} \operatorname{\mathbf{od}}, \sigma, \rho \rangle}$  $\frac{\langle S_0, \sigma, \rho \rangle \to \sum_{i \in I} p_i \cdot \langle S_i, \sigma_i, \rho_i \rangle}{\langle S_0; S_1, \sigma, \rho \rangle \to \sum_{i \in I} p_i \cdot \langle S_i; S_1, \sigma_i, \rho_i \rangle} \text{ where } E; S_1 \equiv S_1$  $\frac{\sigma \models \bigwedge_{j=1}^m \neg B_j}{\langle \mathbf{do} \square_{j=1}^m B_j; \alpha_j \to S_j \ \mathbf{od}, \sigma, \rho \rangle \to \langle E, \sigma, \rho \rangle}$  $(\text{Paral}) \quad \frac{\langle S_k, \sigma, \rho \rangle \to \sum_{i \in I} p_i \cdot \langle S_{k,i}, \sigma_i, \rho_i \rangle, \ 1 \le k \le n}{\langle S_1 \| \dots \| S_k \| \dots \| S_n, \sigma, \rho \rangle \to \sum_{i \in I} p_i \cdot \langle S_1 \| \dots \| S_{k,i} \| \dots \| S_n, \sigma_i, \rho_i \rangle}$  $S_k \equiv \mathbf{do} \ \Box_{j=1}^m B_{k,j}; \alpha_{k,j} \to S_{k,j} \ \mathbf{od}, \quad S_\ell \equiv \mathbf{do} \ \Box_{j=1}^{m'} B_{\ell,j}; \alpha_{\ell,j} \to S_{\ell,j} \ \mathbf{od}, \ 1 \le k < \ell \le n$  $\sigma \models B_{k,j_1} \land B_{\ell,j_2}, \ \alpha_{k,j_1} \text{ and } \alpha_{\ell,j_2} \text{ match}, \textit{Effect}(\alpha_{k,j_1},\alpha_{\ell,j_2}) \equiv x := e, \ 1 \leq j_1 \leq m, 1 \leq j_2 \leq m'$ (Comm) - $\langle S_1 \| \dots \| S_n, \sigma, \rho \rangle \rightarrow \langle S'_1 \| \dots \| S'_n, \sigma[\sigma(e)/x], \rho \rangle$ where  $S'_k \triangleq S_{k,j_1}; S_k, \ S'_{\ell} \triangleq S_{\ell,j_2}; S_{\ell}$ , and  $S'_i \triangleq S_i$  for  $i \neq k, \ell$ 

**Table 1** Operational semantics for distributed quantum programs, where  $\sigma$  is a proper classical state; i.e.,  $\sigma \neq \text{fail}$ .

(2)  $\operatorname{tr}(\Delta) \triangleq \sum_{\sigma \in \lceil \Delta \rceil} \operatorname{tr}[\Delta(\sigma)] \le 1.$ 

Denote by  $qv(\Delta)$  the set V of quantum variables in  $\Delta$  defined in Definition 4. Sometimes it is convenient to denote a cq-state  $\Delta$  by the explicit form  $\bigoplus_{i \in I} \langle \sigma_i, \rho_i \rangle$  where  $\lceil \Delta \rceil = \{\sigma_i : i \in I\}$  and  $\Delta(\sigma_i) = \rho_i$  for each  $i \in I$ . When  $\Delta$  is a simple function such that  $\lceil \Delta \rceil = \{\sigma\}$  for some  $\sigma$  and  $\Delta(\sigma) = \rho$ , we denote  $\Delta$  simply by  $\langle \sigma, \rho \rangle$ . Let  $\{\Delta_i : i \in I\}$  be a countable set of cq-states over V such that for any  $\sigma$ ,  $\sum_{i \in I} \Delta_i(\sigma) = \rho_\sigma$  for some  $\rho_\sigma \in \mathcal{D}(\mathcal{H}_V)$  and  $\sum_{i \in I} \operatorname{tr}(\Delta_i) \leq 1$ . Then the summation of them, denoted  $\sum_{i \in I} \Delta_i$ , is a cq-state  $\Delta$  over V such that for any  $\sigma \in \Sigma$ ,  $\Delta(\sigma) = \rho_\sigma$ . Obviously,  $\lceil \Delta \rceil = \bigcup_{i \in I} \lceil \Delta_i \rceil$ . It is worth noting the difference between  $\sum_{i \in I} \langle \sigma_i, \rho_i \rangle$ , the summation of some (simple) cq-states, and  $\bigoplus_{i \in I} \langle \sigma_i, \rho_i \rangle$ , the explicit form of a single one: in the latter  $\sigma_i$ 's must be distinct while in the former they may not.

Let  $S_V$  be the set of all cq-states over V, and S the set of all cq-states; that is,  $S \triangleq \bigcup_{V \subseteq qVar} S_V$ . We extend the Löwner order  $\sqsubseteq_V$  for  $\mathcal{D}(\mathcal{H}_V)$  pointwisely to S by letting  $\Delta \sqsubseteq \Delta'$  iff  $qv(\Delta) = qv(\Delta')$ and for all  $\sigma \in \Sigma$ ,  $\Delta(\sigma) \sqsubseteq_{qv(\Delta)} \Delta'(\sigma)$ . Then  $S_V$  is a pointed  $\omega$ -CPO under  $\sqsubseteq$ , with the least element being the constant  $\mathbf{0}_{\mathcal{H}_V}$  function, denoted  $\bot_V$ . Furthermore, S as a whole is an  $\omega$ -CPO under  $\sqsubseteq$ . When  $\Delta \sqsubseteq \Delta'$ , there exists a unique  $\Delta'' \in S_{qv(\Delta)}$ , denoted  $\Delta' - \Delta$ , such that  $\Delta'' + \Delta = \Delta'$ . For any real numbers  $\lambda_i$ ,  $i \in I$ , if both  $\Delta_+ \triangleq \sum_{\lambda_i > 0} \lambda_i \Delta_i$  and  $\Delta_- \triangleq \sum_{\lambda_i < 0} (-\lambda_i) \Delta_i$  are well-defined and  $\Delta_- \sqsubseteq \Delta_+$ , then the linear-sum  $\sum_{i \in I} \lambda_i \Delta_i$  is defined to be  $\Delta_+ - \Delta_-$ . In the rest of this paper, whenever we write  $\sum_{i \in I} \lambda_i \Delta_i$  we always assume that it is well-defined. Finally, let  $\mathcal{E}$  be a completely positive and trace-nonincreasing super-operator from  $\mathcal{L}(\mathcal{H}_V)$  to  $\mathcal{L}(\mathcal{H}_W)$ . We extend it to  $S_V$  in a pointwise way:  $\mathcal{E}(\Delta)(\sigma) = \mathcal{E}(\Delta(\sigma))$  for all  $\sigma$ .

# 3.2 Operational Semantics

Let *Prog* be the set of all distributed quantum programs. A *configuration* is a triple  $(S, \sigma, \rho)$  where  $S \in Prog \cup \{E\}$  with E being a special symbol to denote termination,  $\sigma \in \Sigma \cup \{\text{fail}\}$  with fail

being another special symbol to denote the failure state, and  $\rho \in \mathcal{D}(\mathcal{H}_V)$  for some V subsuming qv(S) with tr( $\rho$ ) = 1. We always identify  $E \parallel \ldots \parallel E$  with E. The operational semantics of programs in *Prog* is defined as the smallest transition relation  $\rightarrow$  given in Table 1.

▶ Remark. The transition rules presented in Table 1 for sequential quantum programs follows the same spirit as in [16], except for the newly introduced alternative and repetitive commands whose semantics definitions are also standard [11]. The rules (Paral) and (Comm) are similar to their analogy for classical non-probabilistic programs [1].

It is worth noting that the transitions for quantum measurements and probabilistic assignments in [16] are given in a 'non-deterministic' way, with the probabilities of different branches being encoded in the quantum part of the configurations (by allowing partial density operators instead of density operators in configurations). Note that it is only a matter of notational convenience to represent probabilistic choices with non-determinism. However, distributed quantum programs investigated in this paper exhibit real non-determinism due to the possible interleaving of local actions and communication of different sequential processes. To distinguish these two types of non-determinism, we decide to model quantum measurements and probabilistic assignments in a (standard) probabilistic way.

The following lemma, which can be easily proved by inspecting the transition rules in Table 1, shows that  $\rightarrow$  is indeed a relation from configurations to probability distributions of configurations.

▶ Lemma 5. Let  $(S, \sigma, \rho)$  be a configuration and  $(S, \sigma, \rho) \rightarrow \sum_{i \in I} p_i \cdot \langle S_i, \sigma_i, \rho_i \rangle$ . Then  $\sum_{i \in I} p_i = 0$ 1.

The next lemma extends the Change and Access lemma for classical programs by considering the effects of transitions on quantum states.

▶ Lemma 6 (Change and Access). Let  $(S, \sigma, \rho) \rightarrow \mu$ . Then there exist a set  $\{S_i : i \in I\}$  of distributed programs with  $v(S_i) \subseteq v(S)$  for  $v \in \{change, qv, cv\}$ , a set  $\{f_i : i \in I\}$  of functions over  $\Sigma$ , and a set  $\{\mathcal{E}_i : i \in I\}$  of super-operators acting on  $\mathcal{H}_{qv(S)}$  such that

- (1) for each i,  $f_i$  does not change the value of variables outside change(S). That is, for all  $\tau \in \Sigma$ ,  $f_i(\tau)|_V = \tau|_V$  where  $V \triangleq c Var \setminus change(S)$ ;
- (2) for each *i*,  $f_i$  depends only on cv(S). That is,  $f_i(\sigma)|_{cv(S)} = f_i(\tau)|_{cv(S)}$  whenever  $\sigma|_{cv(S)} = f_i(\tau)|_{cv(S)}$  $\tau|_{cv(S)};$
- (3)  $\sum_{i \in I} \mathcal{E}_i$  is trace-nonincreasing;
- (4)  $\mu = \sum_{i \in I, p_i > 0} p_i \cdot \langle S_i, f_i(\sigma), \mathcal{E}_i(\rho) / p_i \rangle$  where  $p_i = \operatorname{tr}(\mathcal{E}_i(\rho));$ (5) for any  $\sigma'$  which agrees with  $\sigma$  on cv(S), i.e.  $\sigma'|_{cv(S)} = \sigma|_{cv(S)}$ , and  $\rho' \in \mathcal{D}(\mathcal{H}_V)$  with  $V \supseteq qv(S)$ ,

$$\langle S, \sigma', \rho' \rangle \to \sum_{i \in I, p'_i > 0} p'_i \cdot \langle S_i, f_i(\sigma'), \mathcal{E}_i(\rho') / p'_i \rangle \tag{1}$$

where  $p'_i = \operatorname{tr}(\mathcal{E}_i(\rho')).$ 

A configuration is called a terminal if it has no successor distributions. Because of the communication constraints, distributed programs can also end up with a deadlock configuration, in which not all the processes terminate properly (become E), and none of them has led to a failure (the classical state becomes fail). In other words,  $\langle S, \sigma, \rho \rangle$  is a terminal iff  $S \equiv E, \sigma \equiv$  fail, or it is a deadlock. For a distribution  $\mu = \sum_{i \in I} p_i \cdot \langle S_i, \sigma_i, \rho_i \rangle$  of configurations, we denote by

$$\Delta_{\mu} \triangleq \sum_{i \in I, S_i \equiv E, \sigma_i \neq \mathbf{fail}} \langle \sigma_i, p_i \rho_i \rangle$$

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the cq-state obtained by restricting  $\mu$  on the properly terminated configurations. Let  $\Pr_{\mu}(E) \triangleq \operatorname{tr}(\Delta_{\mu})$  be the probability of  $\mu$  having properly terminated.

The transition relation  $\rightarrow$  defined above can be further extended to distributions of configurations by letting  $\mu \rightarrow \nu$  where  $\mu = \sum_{i \in I} p_i \cdot c_i$  if (1) for each  $i, c_i \rightarrow \nu_i$  for some  $\nu_i$  whenever  $c_i$  is not a terminal; otherwise, let  $\nu_i \triangleq c_i$ , and (2)  $\nu = \sum_{i \in I} p_i \cdot \nu_i$ . It is easy to check that such a  $\nu$  is a valid distribution over configurations. Let  $\rightarrow^k$  be the k-fold composition of  $\rightarrow$ , and  $\rightarrow^* \triangleq \bigcup_{k \ge 0} \rightarrow^k$  the reflexive and transitive closure of  $\rightarrow$ .

Let  $S \in Prog$ , and  $\langle \sigma, \rho \rangle \in S_V$  with  $V \supseteq qv(S)$  and  $tr(\rho) = 1$ . A *computation* of S starting in  $\langle \sigma, \rho \rangle$  is an infinite sequence  $\pi \triangleq \{\mu_i : i \ge 0\}$  of distributions over configurations where  $\mu_0 = \langle S, \sigma, \rho \rangle$  and for each  $i \ge 0, \mu_i \to \mu_{i+1}$ .

▶ Lemma 7. Let  $\pi \triangleq \{\mu_i : i \ge 0\}$  be a computation starting in  $\langle \sigma, \rho \rangle$ . Then  $\Delta_{\mu_0} \sqsubseteq \Delta_{\mu_1} \sqsubseteq \ldots$ 

With Lemma 7, we can define for any computation  $\pi \triangleq \{\mu_i : i \ge 0\}$  the cq-state computed by  $\pi$  as  $\Delta_{\pi} \triangleq \bigvee_{i>0} \Delta_{\mu_i}$ , the least upper bound of  $\Delta_{\mu_i}$  according to  $\sqsubseteq$ .

► **Example 8** (Operational Semantics of Quantum Teleportation). Let  $\sigma$  be a classical state and  $|\psi\rangle$  a pure state in  $\mathcal{H}_2$ . Then one of the computations, denoted  $\pi$ , of *Teleport* starting in  $\langle \sigma, |\psi\rangle_q \langle \psi| \otimes |\beta\rangle_{q_1,q_2} \langle \beta| \rangle$  is shown as follows:

$$\langle Teleport, \sigma, [|\psi, \beta\rangle] \rangle$$

$$\rightarrow^{5} \sum_{i,j=0,1} \frac{1}{4} \cdot \langle \mathbf{do}_{a} \| \mathbf{do}_{b}, \sigma[i/x_{A}, j/z_{A}, 0/stage_{A}, 0/stage_{B}, [|j, i, X^{i}Z^{j}\psi\rangle] \rangle$$

$$\rightarrow \sum_{i,j=0,1} \frac{1}{4} \cdot \langle stage_{A} := 1; \mathbf{do}_{a} \| stage_{B} := 1; \mathbf{if} \ x_{B} = 1 \rightarrow q_{2} *= X \square \neg (x_{B} = 1) \rightarrow$$

$$\mathbf{skip}; \ \mathbf{do}_{b}, \sigma[i/x_{A}, j/z_{A}, 0/stage_{A}, 0/stage_{B}, i/x_{B}], [|j, i, X^{i}Z^{j}\psi\rangle] \rangle$$

$$\rightarrow^{4} \sum_{i,j=0,1} \frac{1}{4} \cdot \langle \mathbf{do}_{a} \| \mathbf{do}_{b}, \sigma[i/x_{A}, j/z_{A}, 1/stage_{A}, 1/stage_{B}, i/x_{B}], [|j, i, Z^{j}\psi\rangle] \rangle$$

$$\rightarrow^{5} \sum_{i,j=0,1} \frac{1}{4} \cdot \langle \mathbf{do}_{a} \| \mathbf{do}_{b}, \sigma[i/x_{A}, j/z_{A}, 2/stage_{A}, 2/stage_{B}, i/x_{B}, j/z_{B}], [|j, i, \psi\rangle] \rangle$$

$$\rightarrow^{2} \mu \triangleq \sum_{i,j=0,1} \frac{1}{4} \cdot \langle E, \sigma[i/x_{A}, j/z_{A}, 2/stage_{A}, 2/stage_{B}, i/x_{B}, j/z_{B}], [|j, i, \psi\rangle] \rangle$$

$$\rightarrow \mu \rightarrow \cdots$$

where  $\mathbf{do}_a$  and  $\mathbf{do}_b$  are the **do**-loops of *Alice* and *Bob*, respectively. For pure state  $|\phi\rangle$ , we denote by  $[|\phi\rangle]$  its corresponding density operator  $|\phi\rangle\langle\phi|$ . Thus

$$\Delta_{\pi} = \sum_{i,j=0,1} \left\langle \sigma[i/x_A, j/z_A, 2/stage_A, 2/stage_B, i/x_B, j/z_B], \frac{1}{4}[|j, i, \psi\rangle] \right\rangle.$$

Note that although each component process of a distributed program is deterministic, the whole program can still exhibit nondeterminism. This is due to the interleaving nature of local actions of individual processes and communication between disjoint pairs of processes; see Rules (Paral) and (Comm) in Table 1. However, the following theorem shows that these different computations actually compute the same cq-state.

▶ **Theorem 9** (Determinism). Let  $S \in Prog$  be a distributed quantum program, and  $\langle \sigma, \rho \rangle \in S_V$  with  $V \supseteq qv(S)$  and  $tr(\rho) = 1$ . Then the set

 $\{\Delta_{\pi} : \pi \text{ is a computation of } S \text{ starting in } \langle \sigma, \rho \rangle \}$ 

has exactly one element.

# 3.3 Denotational Semantics

With Theorem 9, the denotational semantics of distributed quantum programs can be defined using the operational one. Let  $S_{\supseteq qv(S)} \triangleq \bigcup_{V \supset qv(S)} S_V$ .

▶ **Definition 10.** Let  $S \in Prog$ . The *denotational semantics* of S is a mapping  $\llbracket S \rrbracket : S_{\supseteq qv(S)} \to S_{\supseteq qv(S)}$  such that

(1) for any  $\langle \sigma, \rho \rangle \in \mathcal{S}_V$  with  $V \supseteq qv(S)$  and  $\operatorname{tr}(\rho) = 1$ ,

 $[[S]](\sigma,\rho) \triangleq \text{ the unique element in } \{\Delta_{\pi} : \pi \text{ is a computation of } S \text{ starting in } \langle \sigma, \rho \rangle \};$ 

(2) for any  $\Delta = \bigoplus_{i \in I} \langle \sigma_i, \rho_i \rangle$  (thus  $\operatorname{tr}(\rho_i) > 0$  for any  $i \in I$ ),

$$\llbracket S \rrbracket(\Delta) \triangleq \sum_{i \in I} \operatorname{tr}(\rho_i) \cdot \llbracket S \rrbracket \left( \sigma_i, \frac{\rho_i}{\operatorname{tr}(\rho_i)} \right).$$

To simplify notation, we always write  $(\sigma, \rho)$  for  $(\langle \sigma, \rho \rangle)$  when  $\langle \sigma, \rho \rangle$  appears as a parameter of some function. The next lemma guarantees the well-definedness of Definition 10.

▶ Lemma 11. Let  $S \in Prog and \Delta \in S_V$  with  $V \supseteq qv(S)$ . Then (1)  $[[S]](\Delta)$  has countable support, and  $tr([[S]](\Delta)) \le tr(\Delta)$ . Hence  $[[S]](\Delta) \in S_V$  as well; (2) for any  $\lambda_i \in \mathbb{R}$ ,  $[[S]](\Delta) = \sum_i \lambda_i \cdot [[S]](\Delta_i)$  whenever  $\Delta = \sum_i \lambda_i \cdot \Delta_i$ .

# 4 Transformation to sequential quantum programs

Throughout this section, we consider a distributed quantum program  $S \triangleq S_1 \| \cdots \| S_n$  where for each i,

$$S_i \triangleq S_{i,0}$$
; **do**  $\Box_{j=1}^{m_i} B_{i,j}$ ;  $\alpha_{i,j} \to S_{i,j}$  **od**.

The transformation of S into a sequential one follows the standard approach for classical (non-probabilistic) programs [1].

Let  $\Gamma \triangleq \{(i, j, k, \ell) : \alpha_{i,j} \text{ and } \alpha_{k,\ell} \text{ match, and } i < k\}$ . That is,  $\Gamma$  collects all the pairs of generalised guards in the component processes which are able to communicate. The *sequentialisation* of S is defined as

$$T(S) \triangleq S_{1,0}; \dots; S_{n,0};$$
  
**do**  $\Box_{(i,j,k,\ell)\in\Gamma} B_{i,j} \land B_{k,\ell} \land B_i \to Effect(\alpha_{i,j}, \alpha_{k,\ell}); S_{i,j}; S_{k,\ell}$   
**od**

where  $B_i \triangleq \bigwedge_{(t,j,k,\ell)\in\Gamma,t\leq i} \neg (B_{t,j} \land B_{k,\ell})$ . When  $\Gamma$  is empty, we simply drop the **do** loop in the definition.

Note that we introduce an additional condition  $B_i$  here to guarantee that the resultant quantum program is deterministic (so that it can be described in the language presented in Sec. 2.1). This is unnecessary for classical programs in [1], since verification of nondeterministic classical programs has been well investigated. However, from Theorem 9 the nondeterministic choices in S do not really matter in computing the final cq-state. Therefore, introducing the additional condition  $B_i$  does not put any restriction on the expressiveness of the sequentialised program T(S); this will be more rigorously shown with Theorem 12 below.

It is obvious that S and T(S) are not semantically equivalent: at least they have different conditions for termination. To see this, let

$$TERM \triangleq \bigwedge_{i=1}^{n} \bigwedge_{j=1}^{m_{i}} \neg B_{i,j}, \quad BLOCK \triangleq \bigwedge_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell}) = \bigwedge_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{k,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{i,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{i,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{i,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{i,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{i,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{i,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{i,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{i,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{i,\ell} \land B_{i,\ell}) = \sum_{(i,j,k,\ell) \in \Gamma} \neg (B_{i,j} \land B_{i,\ell}) = \sum_{(i,j,\ell) \in \Gamma} \neg (B_{i,j} \land B_{i,\ell})$$

Then S terminates iff TERM holds while T(S) terminates iff BLOCK holds. Note that  $TERM \rightarrow$ *BLOCK* but generally the reverse direction is not true.

The following theorem shows that S and T(S) are indeed equivalent conditioning on TERM.

▶ **Theorem 12.** For any cq-state  $\Delta \in S_V$  with  $V \supseteq qv(S)$ ,  $[[S]](\Delta) = [[T(S)]](\Delta)|_{TERM}$ , the restriction of  $\llbracket T(S) \rrbracket (\Delta)$  on the set of classical states  $\sigma$  with  $\sigma \models TERM$ .

**Example 13** (Sequentialisation of Teleportation). The sequentialisation of *Teleport*, denoted T(Teleport), is as follows:

$$\begin{array}{l} q,q_1 \mathrel{*=} CNOT; \ q \mathrel{*=} H; \ z_A \mathrel{:=} \mathbf{meas} \ q; \ x_A \mathrel{:=} \mathbf{meas} \ q_1; \\ stage_A \mathrel{:=} 0; \ stage_B \mathrel{:=} 0; \\ \mathbf{do} \ stage_A = 0 \land stage_B = 0 \rightarrow x_B \mathrel{:=} x_A; \\ stage_A \mathrel{:=} 1; \ stage_B \mathrel{:=} 1; \ \mathbf{if} \ x_B = 1 \rightarrow \ q_2 \mathrel{*=} X \square \neg (x_B = 1) \rightarrow \mathbf{skip} \ \mathbf{fi} \\ \square \ stage_A = 1 \land stage_B = 1 \rightarrow z_B \mathrel{:=} z_A; \\ stage_A \mathrel{:=} 2; \ stage_B \mathrel{:=} 2; \ \mathbf{if} \ z_B = 1 \rightarrow \ q_2 \mathrel{*=} Z \square \neg (z_B = 1) \rightarrow \mathbf{skip} \ \mathbf{fi} \\ \mathbf{od} \end{array}$$

oa

It is easy to see that

 $\llbracket Teleport \rrbracket(\Delta) = \llbracket T(Teleport) \rrbracket(\Delta)|_{stage_A \notin \{0,1\} \land stage_B \notin \{0,1\}}.$ 

#### 5 Verification of distributed quantum programs

The basic notion for verification of distributed quantum programs is classical-quantum assertion from [16].

#### 5.1 **Classical-quantum assertions**

Recall that assertions for classical program states are usually represented as first order logic formulas over *cVar*. For any classical assertion *p*, denote by  $[[p]] \triangleq \{\sigma \in \Sigma : \sigma \models p\}$  the set of classical states that satisfy p. Two assertions p and p' are equivalent, written  $p \equiv p'$ , iff [[p]] = [[p']]. Let  $\mathcal{P}(\mathcal{H}_V)$  be the set of Hermitian operators on  $\mathcal{H}$  whose eigenvalues lie between 0 and 1.

▶ Definition 14. Given  $V \subseteq qVar$ , a *classical-quantum assertion* (cq-assertion for short)  $\Theta$  over V is a function in  $\Sigma \to \mathcal{P}(\mathcal{H}_V)$  such that

- (1) the image set  $\Theta(\Sigma)$  of  $\Theta$  is countable;
- (2) for each  $M \in \Theta(\Sigma)$ , the preimage  $\Theta^{-1}(M)$  is definable by a classical assertion p in the sense that  $[\![p]\!] = \Theta^{-1}(M).$

Denote by  $qv(\Theta)$  the set V of quantum variables in  $\Theta$ . We write  $\bigoplus_{i \in I} \langle p_i, M_i \rangle$  instead of  $\bigoplus_{i \in I} \langle \llbracket p_i \rrbracket, M_i \rangle$  for a cq-assertion  $\Theta$  whenever  $\Theta(\Sigma) = \{M_i : i \in I\}$  and  $\Theta^{-1}(M_i) = \llbracket p_i \rrbracket$  for each  $i \in I$ . Note that this representation is not unique: the representative assertion  $p_i$  can be replaced by  $p'_i$  whenever  $p_i \equiv p'_i$ . Furthermore, the summand with zero operator  $\mathbf{0}_{\mathcal{H}_V}$  is always omitted. In

particular, when  $\Theta(\Sigma) = {\mathbf{0}_{\mathcal{H}}, M}$  or  ${M}$  for some  $M \neq \mathbf{0}_{\mathcal{H}_V}$ , we simply denote  $\Theta$  by  $\langle p, M \rangle$  for some p with  $\Theta^{-1}(M) = [[p]]$ .

Let  $\mathcal{A}_V$  be the set of all cq-assertions over V, and  $\mathcal{A}$  the set of all cq-assertions. Again, we extend the Löwner order  $\sqsubseteq_V$  for  $\mathcal{L}(\mathcal{H}_V)$  pointwisely to  $\mathcal{A}$  by letting  $\Theta \sqsubseteq \Theta'$  iff  $qv(\Theta) = qv(\Theta')$  and for all  $\sigma \in \Sigma, \Theta(\sigma) \sqsubseteq_{qv(\Theta)} \Theta'(\sigma)$ . It is easy to see that  $\mathcal{A}_V$  is also a pointed  $\omega$ -CPO under  $\sqsubseteq$ , with the least element being  $\bot_V$ . Furthermore, it has the largest element  $\top_V \triangleq \langle \mathbf{true}, I_{\mathcal{H}_V} \rangle$ . When  $\Theta \sqsubseteq \Theta'$ , we denote by  $\Theta' - \Theta$  the unique  $\Theta'' \in \mathcal{A}_{qv(\Theta)}$  such that  $\Theta'' + \Theta = \Theta'$ . With these notions, summation and linear-sum of cq-assertions can be defined similarly as for cq-states. Let  $V_1, V_2$  be two subsets of qVar, and  $\Theta_i \in \mathcal{A}_{V_i}$ , i = 1, 2. We say  $\Theta_1 \lesssim \Theta_2$  whenever  $\Theta_1 \otimes I_{\mathcal{H}_{V_2\setminus V_1}} \sqsubseteq I_{\mathcal{H}_{V_1\setminus V_2}} \otimes \Theta_2$ . Obviously, when restricted on some given set of quantum variables,  $\lesssim$  coincides with  $\sqsubseteq$ .

Given a classical assertion p, we denote by  $p \bowtie \sum_i \langle p_i, M_i \rangle$  the cq-assertion  $\sum_i \langle p \bowtie p_i, M_i \rangle$ (if it is valid) where  $\bowtie$  can be any logic connective such as  $\land, \lor, \Rightarrow, \Leftrightarrow$ , etc. Let  $\mathcal{F}$  be a completely positive and sub-unital linear map from  $\mathcal{P}(\mathcal{H}_V)$  to  $\mathcal{P}(\mathcal{H}_W)$ . We extend it to  $\mathcal{A}_V$  in a pointwise way. In particular, when  $qv(\Theta) \cap W = \emptyset, \Theta \otimes I_{\mathcal{H}_W}$  is a cq-assertion which maps any  $\sigma \in \Sigma$  to  $\Theta(\sigma) \otimes I_{\mathcal{H}_W}$ .

▶ **Definition 15.** Given a cq-state  $\Delta$  and a cq-assertion  $\Theta$  with  $qv(\Delta) \supseteq qv(\Theta)$ , the *expectation* of  $\Delta$  satisfying  $\Theta$  is defined to be

$$\operatorname{Exp}(\Delta \models \Theta) \triangleq \sum_{\sigma \in \lceil \Delta \rceil} \operatorname{tr} \left[ (\Theta(\sigma) \otimes I_{\mathcal{H}_{V}}) \cdot \Delta(\sigma) \right] = \sum_{\sigma \in \lceil \Delta \rceil} \operatorname{tr} \left[ \Theta(\sigma) \cdot \operatorname{tr}_{\mathcal{H}_{V}}(\Delta(\sigma)) \right]$$

where  $V = qv(\Delta) \setminus qv(\Theta)$  and the dot  $\cdot$  denotes matrix multiplication.

### 5.2 Correctness formula

As usual, program correctness is expressed by *correctness formulas* with the form  $\{\Theta\} \ S \ \{\Psi\}$  where S is a distribute quantum program, and  $\Theta$  and  $\Psi$  are both cq-assertions. We do not put any requirement on the quantum variables which  $\Theta$  and  $\Psi$  are acting on. In fact, the sets qv(S),  $qv(\Theta)$ , and  $qv(\Psi)$  can be all different.

**Definition 16.** Let  $S \in Prog$ , and  $\Theta$  and  $\Psi$  be cq-assertions.

(1) We say the correctness formula  $\{\Theta\} \ S \ \{\Psi\}$  is true in the sense of *total correctness*, written  $\models_{tot} \{\Theta\} \ S \ \{\Psi\}$ , if for any  $V \supseteq qv(S, \Theta, \Psi)$  and  $\Delta \in S_V$ ,

$$\operatorname{Exp}(\Delta \models \Theta) \le \operatorname{Exp}(\llbracket S \rrbracket(\Delta) \models \Psi).$$

(2) We say the correctness formula  $\{\Theta\} \ S \ \{\Psi\}$  is true in the sense of *partial correctness*, written  $\models_{par} \{\Theta\} \ S \ \{\Psi\}$ , if for any  $V \supseteq qv(S, \Theta, \Psi)$  and  $\Delta \in S_V$ ,

$$\operatorname{Exp}(\Delta \models \Theta) \le \operatorname{Exp}(\llbracket S \rrbracket(\Delta) \models \Psi) + \operatorname{tr}(\Delta) - \operatorname{tr}(\llbracket S \rrbracket(\Delta)).$$

**Example 17.** The correctness of quantum teleportation can be stated as follows: for any  $|\psi\rangle \in \mathcal{H}_2$ ,

 $\models_{tot} \{ |\psi\rangle_q \otimes |\beta\rangle_{q_1,q_2} \} \ Teleport \ \{ |\psi\rangle_{q_2} \},$ 

which claims that the (arbitrary) quantum state of qubit q is successfully transmitted to qubit  $q_2$  by *Teleport*. Note that the postcondition  $|\psi\rangle_{q_2}$  does not refer to q and  $q_1$ , meaning that the postmeasurement state of these quantum systems is irrelevant.



where  $\Gamma$  and *TERM* are defined as in Sec. 4.

**Table 2** Proof system for partial correctness.

# 5.3 Proof systems

The core of Hoare logic is a proof system consisting of axioms and proof rules which enable syntaxoriented and modular reasoning of program correctness. In this section, we propose a Hoare logic for distributed quantum programs.

**Partial correctness**. We propose in Table 2 a proof system for partial correctness of distributed quantum programs, which is a natural extension of the quantum Hoare logic introduced in [16] for deterministic while programs. We write  $\vdash_{par} \{\Theta\} S \{\Psi\}$  if the correctness formula  $\{\Theta\} S \{\Psi\}$  can be derived from the system.

► **Theorem 18.** *The proof system in Table 2 is both sound and (relatively) complete with respect to the partial correctness of distributed quantum programs.* 

**Total correctness.** Ranking functions play a central role in proving total correctness of while loop programs. Recall that in the classical case, a ranking function maps each reachable state in the loop body to an element of a well-founded ordered set (say, the set  $\mathbb{N}$  of nonnegative integers), such that the value decreases strictly after each iteration of the loop. Our proof rules for total correctness of repetitive commands and distributed quantum programs also heavily relies on the notion of ranking assertions.

▶ **Definition 19.** Let  $\Theta \in \mathcal{A}_V$ . A decreasing sequence (w.r.t.  $\sqsubseteq$ ) of cq-assertions  $\{\Theta_k : k \ge 0\}$  in  $\mathcal{A}_V$  with  $\Theta \sqsubseteq \Theta_0$  and  $\bigwedge_k \Theta_k = \bot_V$  are  $\Theta$ -ranking assertions for do  $\Box_{i=1}^n B_i \to S_i$  od if for any  $k \ge 0, 1 \le i \le n$ , and  $\Delta \in \mathcal{S}_W, W \triangleq \bigcup_{i=1}^n qv(S_i) \cup V$ ,

$$\operatorname{Exp}(\llbracket S_i \rrbracket(\Delta|_{B_i}) \models \Theta_k) \le \operatorname{Exp}(\Delta \models \Theta_{k+1}).$$
<sup>(2)</sup>

They are said to be  $\Theta$ -ranking assertions for  $S_1 \parallel \ldots \parallel S_n$  if, for any  $k \ge 0$ ,  $(i, j, t, \ell) \in \Gamma$ , and  $\Delta \in S_W, W \triangleq \bigcup_{i=1}^n qv(S_i) \cup V$ , we have

$$\operatorname{Exp}(\llbracket S_{i,j}^{t,\ell} \rrbracket(\Delta|_{B_{i,j} \wedge B_{t,\ell}}) \models \Theta_k) \le \operatorname{Exp}(\Delta \models \Theta_{k+1})$$

where  $S_{i,j}^{t,\ell} \triangleq Effect(\alpha_{i,j}, \alpha_{t,\ell}); S_{i,j}; S_{t,\ell}.$ 

$$\begin{array}{ll} \text{(Abort-T)} & \{\perp_{V}\} \text{ abort } \{\perp_{V}\} \\ \text{(Alt-T)} & \frac{\Theta \lesssim \bigvee_{i=1}^{n} B_{i}, \{B_{i} \land \Theta\} \ S_{i} \ \{\Psi\}, \forall i \in \{1, \ldots, n\}}{\{\Theta\} \ \text{if } \Box_{i=1}^{n} B_{i} \rightarrow S_{i} \ \text{fi} \ \{\Psi\}} \\ \text{(Rep-T)} & \frac{\{B_{i} \land \Theta\} \ S_{i} \ \{\Theta\}, \forall i \in \{1, \ldots, n\}}{\Theta\text{-ranking assertions exist for } \text{do } \Box_{i=1}^{n} B_{i} \rightarrow S_{i} \ \text{od}}{\{\Theta\} \ \text{do } \Box_{i=1}^{n} B_{i} \rightarrow S_{i} \ \text{od}} \ \left\{\Theta\} \ S_{1,0}; \ldots; S_{n,0} \ \{\Psi\}, \text{and } \Psi\text{-ranking assertions exist for } S_{1} \| \ldots \| S_{i} \\ \frac{\{\Theta\} \ S_{1,0}; \ldots; S_{n,0} \ \{\Psi\}, \text{and } \Psi\text{-ranking assertions exist for } S_{1} \| \ldots \| S_{i} \\ \frac{\{\Theta\} \ S_{1,0}; \ldots; S_{n,0} \ \{\Psi\}, \text{effect}(\alpha_{i,j}, \alpha_{k,\ell}); S_{i,j}; S_{k,\ell} \ \{\Psi\}, \forall (i,j,k,\ell) \in \Pi \\ \Psi \land BLOCK \lesssim TERM \\ \end{array}$$

where  $\Gamma$  and *TERM* are defined as in Sec. 4.

**Table 3** Some proof rules for total correctness.

The proof system for total correctness is then defined as for partial correctness, except that the rules (Abort), (Alt), (Rep), and (Dist) are replaced by their corresponding total correctness version shown in Table 3. We write  $\vdash_{tot} \{\Theta\} S \{\Psi\}$  if the correctness formula  $\{\Theta\} S \{\Psi\}$  can be derived using this proof system.

► **Theorem 20.** *The proof system for total correctness is both sound and (relatively) complete with respect to the total correctness of distributed quantum programs.* 

# 6 Conclusion and future works

In this paper, we propose a distributed programming language for the purpose of formal description and verification of distributed quantum systems. A Hoare-style logic, which turns out to be sound and (relatively) complete for both partial and total correctness, is introduced to help analysis of quantum programs written in this language. Effectiveness of the logic is demonstrated by its application in verification of quantum teleportation and local implementation of non-local CNOT gates, two important protocols widely used in distributed quantum systems.

The distributed language investigated in this paper only allows local quantum operations and classical communication (LOCC). Although LOCC is a widely used quantum communication model, there are also important quantum communication protocols, such as Quantum Key Distribution [4] and Quantum Leader Election [34], which do require transmission of quantum states. It is well known that this kind of quantum communication can be achieved by employing the teleportation protocol (provided that enough entanglement is pre-shared between relevant parties), and thus in principle these protocols can be verified using the logic presented in this paper, but their verification in this way will be clumsy and inconvenient. Therefore, it is desirable to extend our language to include quantum communication in future works. To this end, we have to trace the ownership of each quantum system so that the no-cloning property [38] of quantum information is not violated. We expect that the verification of such distributed quantum programs will be much more challenging.

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# A Preliminaries

This section is devoted to fixing some notations from linear algebra and quantum mechanics that will be used in this paper. For a thorough introduction of relevant backgrounds, we refer to [28, Chapter 2].

# A.1 Basic linear algebra

Let  $\mathcal{H}$  be a Hilbert space. In the finite-dimensional case which we are concerned with here, it is merely a complex linear space equipped with an inner product. Consequently, it is isomorphic to  $\mathbb{C}^d$ where  $d = \dim(\mathcal{H})$ , the dimension of  $\mathcal{H}$ . Following the tradition in quantum computing, vectors in  $\mathcal{H}$  are denoted in the Dirac form  $|\psi\rangle$ . The inner product of  $|\psi\rangle$  and  $|\phi\rangle$  is written  $\langle \psi | \phi \rangle$ , and they are *orthogonal* if  $\langle \psi | \phi \rangle = 0$ . The *outer product* of them, denoted  $|\psi\rangle \langle \phi|$ , is a rank-one linear operator which maps any  $|\psi'\rangle$  in  $\mathcal{H}$  to  $\langle \phi | \psi' \rangle | \psi \rangle$ . The *length* of  $|\psi\rangle$  is defined to be  $|||\psi\rangle|| \triangleq \sqrt{\langle \psi | \psi \rangle}$  and it is called *normalised* if  $|||\psi\rangle|| = 1$ . A set of vectors  $B \triangleq \{|i\rangle : i \in I\}$  in  $\mathcal{H}$  is *orthonormal* if each  $|i\rangle$ is normalised and every two of them are orthogonal. Furthermore, if they span the whole space  $\mathcal{H}$ ; that is, any vector in  $\mathcal{H}$  can be written as a linear combination of vectors in B, then B is called an *orthonormal basis* of  $\mathcal{H}$ .

Let  $\mathcal{L}(\mathcal{H})$  be the set of linear operators on  $\mathcal{H}$ , and  $\mathbf{0}_{\mathcal{H}}$  and  $I_{\mathcal{H}}$  the zero and identity operators respectively. Let  $A \in \mathcal{L}(\mathcal{H})$ . The *trace* of A is defined to be  $\operatorname{tr}(A) \triangleq \sum_{i \in I} \langle i|A|i \rangle$  for some (or, equivalently, any) orthonormal basis  $\{|i\rangle : i \in I\}$  of  $\mathcal{H}$ . The *adjoint* of A, denoted  $A^{\dagger}$ , is the unique linear operator in  $\mathcal{L}(\mathcal{H})$  such that  $\langle \psi|A|\phi \rangle = \langle \phi|A^{\dagger}|\psi \rangle^*$  for all  $|\psi \rangle, |\phi \rangle \in \mathcal{H}$ . Here for a complex number  $z, z^*$  denotes its conjugate. Operator A is said to be *normal* if  $A^{\dagger}A = AA^{\dagger}$ , *hermitian* if  $A^{\dagger} = A$ , *unitary* if  $A^{\dagger}A = I_{\mathcal{H}}$ , and *positive* if for all  $|\psi \rangle \in \mathcal{H}, \langle \psi|A|\psi \rangle \ge 0$ . Obviously, hermitian operators are normal, and both unitary operators and positive ones are hermitian. Any normal operator A can be written into a *spectral decomposition* form  $A = \sum_{i \in I} \lambda_i |i\rangle \langle i|$  where  $\{|i\rangle : i \in I\}$  constitute some orthonormal basis of  $\mathcal{H}$ . Furthermore, if A is hermitian, then all  $\lambda_i$ 's are real; if A is unitary, then all  $\lambda_i$ 's have unit length; if A is positive, then all  $\lambda_i$ 's are non-negative. The Löwner (partial) order  $\sqsubseteq_{\mathcal{H}}$  on the set of hermitian operators on  $\mathcal{H}$  is defined by letting  $A \sqsubseteq_{\mathcal{H}} B$  iff B - A is positive.

Let  $\mathcal{H}_1$  and  $\mathcal{H}_2$  be two finite dimensional Hilbert spaces, and  $\mathcal{H}_1 \otimes \mathcal{H}_2$  their tensor product. Let  $A_i \in \mathcal{L}(\mathcal{H}_i)$ . The tensor product of  $A_1$  and  $A_2$ , denoted  $A_1 \otimes A_2$  is a linear operator in  $\mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$  such that  $(A_1 \otimes A_2)|(\psi_1\rangle \otimes |\psi_2\rangle\rangle = (A_1|\psi_1\rangle) \otimes (A_2|\psi_2\rangle)$  for all  $|\psi_i\rangle \in \mathcal{H}_i$ . To simplify notations, we often write  $|\psi_1\rangle|\psi_2\rangle$  for  $|\psi_1\rangle \otimes |\psi_2\rangle$ . Given  $\mathcal{H}_1$  and  $\mathcal{H}_2$ , the *partial trace* with respect to  $\mathcal{H}_2$ , denoted  $\operatorname{tr}_{\mathcal{H}_2}$ , is a linear mapping from  $\mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$  to  $\mathcal{L}(\mathcal{H}_1)$  such that for any  $|\psi_i\rangle, |\phi_i\rangle \in \mathcal{H}_i$ , i = 1, 2,

$$\operatorname{tr}_{\mathcal{H}_2}(|\psi_1\rangle\langle\phi_1|\otimes|\phi_1\rangle\langle\phi_2|) = \langle\phi_2|\phi_1\rangle|\psi_1\rangle\langle\phi_1|.$$

The definition is extended to  $\mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$  by linearity.

A linear operator  $\mathcal{E}$  from  $\mathcal{L}(\mathcal{H}_1)$  to  $\mathcal{L}(\mathcal{H}_2)$  is called a *super-operator*. It is said to be (1) *positive* if it maps positive operators to positive operators; (2) *completely positive* if all the cylinder extension  $\mathcal{I}_{\mathcal{H}} \otimes \mathcal{E}$  is positive for all finite dimensional Hilbert space  $\mathcal{H}$ , where  $\mathcal{I}_{\mathcal{H}}$  is the identity superoperator on  $\mathcal{L}(\mathcal{H})$ ; (3) *trace-preserving* (resp. *trace-nonincreasing*) if  $tr(\mathcal{E}(A)) = tr(A)$  (resp.  $tr(\mathcal{E}(A)) \leq tr(A)$  for any positive operator  $A \in \mathcal{L}(\mathcal{H}_1)$ ; (4) *unital* (resp. *sub-unital*) if  $\mathcal{E}(I_{\mathcal{H}_1}) = I_{\mathcal{H}_2}$  (resp.  $\mathcal{E}(I_{\mathcal{H}_1}) \sqsubseteq_{\mathcal{H}_2} I_{\mathcal{H}_2}$ ). From *Kraus representation theorem* [27], a super-operator  $\mathcal{E}$  from  $\mathcal{L}(\mathcal{H}_1)$  to  $\mathcal{L}(\mathcal{H}_2)$  is completely positive iff there is some set of linear operators, called *Kraus operators*,  $\{E_i : i \in I\}$  from  $\mathcal{H}_1$  to  $\mathcal{H}_2$  such that  $\mathcal{E}(A) = \sum_{i \in I} E_i A E_i^{\dagger}$  for all  $A \in \mathcal{L}(\mathcal{H}_1)$ . It is easy to check that the trace and partial trace operations defined above are both completely positive and trace-preserving super-operators. Given a completely positive super-operator  $\mathcal{E}$  from  $\mathcal{L}(\mathcal{H}_1)$  to  $\mathcal{L}(\mathcal{H}_2)$  with Kraus operators.  $\{E_i : i \in I\}$ , the adjoint of  $\mathcal{E}$ , denoted  $\mathcal{E}^{\dagger}$ , is a completely positive super-operator from  $\mathcal{L}(\mathcal{H}_2)$  back to  $\mathcal{L}(\mathcal{H}_1)$  with Kraus operators  $\{E_i^{\dagger} : i \in I\}$ . Then we have  $(\mathcal{E}^{\dagger})^{\dagger} = \mathcal{E}$ , and  $\mathcal{E}$  is trace-preserving (resp. trace-nonincreasing) iff  $\mathcal{E}^{\dagger}$  is unital (resp. sub-unital). Furthermore, for any  $A \in \mathcal{L}(\mathcal{H}_1)$  and  $B \in \mathcal{L}(\mathcal{H}_2)$ ,  $\operatorname{tr}(\mathcal{E}(A) \cdot B) = \operatorname{tr}(A \cdot \mathcal{E}^{\dagger}(B))$ .

# A.2 Basic quantum mechanics

According to von Neumann's formalism of quantum mechanics [36], any quantum system with finite degrees of freedom is associated with a finite-dimensional Hilbert space  $\mathcal{H}$  called its *state space*. When dim( $\mathcal{H}$ ) = 2, we call such a system a *qubit*, the analogy of bit in classical computing. A *pure state* of the system is described by a normalised vector in  $\mathcal{H}$ . When the system is in one of an ensemble of states  $\{|\psi_i\rangle : i \in I\}$  with respective probabilities  $p_i$ , we say it is in a *mixed* state, represented by the *density operator*  $\sum_{i \in I} p_i |\psi_i\rangle \langle \psi_i|$  on  $\mathcal{H}$ . Obviously, a density operator is positive and has trace 1. Conversely, by spectral decomposition, any positive operator with unit trace corresponds to some (not necessarily unique) mixed state.

The state space of a composite system (for example, a quantum system consisting of multiple qubits) is the tensor product of the state spaces of its components. For a mixed state  $\rho$  in  $\mathcal{H}_1 \otimes \mathcal{H}_2$ , partial traces of  $\rho$  have explicit physical meanings: the density operators  $\operatorname{tr}_{\mathcal{H}_1}(\rho)$  and  $\operatorname{tr}_{\mathcal{H}_2}(\rho)$  are exactly the reduced quantum states of  $\rho$  on the second and the first component systems, respectively. Note that in general, the state of a composite system cannot be decomposed into tensor product of the reduced states on its component systems. A well-known example is the 2-qubit state  $|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ . This kind of state is called *entangled state*, and usually is the key to many quantum information processing tasks such as teleportation [5] and superdense coding [6].

The *evolution* of a closed quantum system is described by a unitary operator on its state space: if the states of the system at times  $t_1$  and  $t_2$  are  $\rho_1$  and  $\rho_2$ , respectively, then  $\rho_2 = U\rho_1 U^{\dagger}$  for some unitary operator U which depends only on  $t_1$  and  $t_2$ . In contrast, the general dynamics which can occur in a physical system is described by a completely positive and trace-preserving super-operator on its state space. Note that the unitary transformation  $\mathcal{E}_U(\rho) \triangleq U\rho U^{\dagger}$  is such a super-operator.

A quantum measurement  $\mathcal{M}$  is described by a collection  $\{M_i : i \in I\}$  of linear operators on  $\mathcal{H}$ , where I is the set of measurement outcomes. It is required that the measurement operators satisfy the completeness equation  $\sum_{i \in I} M_i^{\dagger} M_i = I_{\mathcal{H}}$ . If the system is in state  $\rho$ , then the probability that measurement result i occurs is given by  $p_i = \operatorname{tr}(M_i^{\dagger} M_i \rho)$ , and the state of the post-measurement system is  $\rho_i = M_i \rho M_i^{\dagger} / p_i$  whenever  $p_i > 0$ . Note that the super-operator

$$\mathcal{E}_{\mathcal{M}}: \rho \mapsto \sum_{i \in I} p_i \rho_i = \sum_{i \in I} M_i \rho M_i^{\dagger}$$

which maps the initial state to the final (mixed) one when the measurement outcome is ignored is completely positive and trace-preserving. A particular case of measurement is *projective measurement* which is usually represented by a hermitian operator M in  $\mathcal{L}(\mathcal{H})$  called *observable*. Let

$$M = \sum_{m \in spec(M)} m P_m$$

where spec(M) is the set of eigenvalues of M, and  $P_m$  the projection onto the eigenspace associated with m. Obviously, the projectors  $\{P_m : m \in spec(M)\}$  form a quantum measurement.

In this paper, we are especially concerned with the set

$$\mathcal{P}(\mathcal{H}) \triangleq \{ M \in \mathcal{L}(\mathcal{H}) : \mathbf{0}_{\mathcal{H}} \sqsubseteq M \sqsubseteq I_{\mathcal{H}} \}$$

of observables whose eigenvalues lie between 0 and 1, where  $\sqsubseteq$  is the Löwner order on  $\mathcal{L}(\mathcal{H})$ . Furthermore, following Selinger's convention [32], we regard the set of *partial density operators* 

$$\mathcal{D}(\mathcal{H}) \triangleq \{ \rho \in \mathcal{L}(\mathcal{H}) : \mathbf{0}_{\mathcal{H}} \sqsubseteq \rho, \operatorname{tr}(\rho) \le 1 \}$$

as (unnormalised) quantum states. Intuitively, the partial density operator  $\rho$  means that the legitimate quantum state  $\rho/\operatorname{tr}(\rho)$  is reached with probability  $\operatorname{tr}(\rho)$ . As a matter of fact, we note that  $\mathcal{D}(\mathcal{H}) \subseteq \mathcal{P}(\mathcal{H})$ .

# B Some useful lemmas

We first recall some basic properties of cq-states and cq-assertions from [16].

▶ Lemma 21 (Lemma 3.9, [16]). For any cq-state  $\Delta \in S_V$ , cq-assertion  $\Theta \in A_W$  with  $W \subseteq V$ , and classical assertion p,

- (1)  $\operatorname{Exp}(\Delta \models \Theta) \in [0, 1];$
- (2)  $\operatorname{Exp}(\bot_V \models \Theta) = \operatorname{Exp}(\Delta \models \bot_W) = 0, \operatorname{Exp}(\Delta \models \top_W) = \operatorname{tr}(\Delta);$
- (3)  $\operatorname{Exp}(\Delta \models \Theta) = \sum_{i} \lambda_{i} \operatorname{Exp}(\Delta \models \Theta_{i})$  if  $\Theta = \sum_{i} \lambda_{i} \Theta_{i}$ ;
- (4)  $\operatorname{Exp}(\Delta \models \Theta) = \sum_{i} \lambda_i \operatorname{Exp}(\Delta_i \models \Theta)$  if  $\Delta = \sum_{i} \lambda_i \Delta_i$ ;
- (5)  $\operatorname{Exp}(\Delta|_p \models \Theta) = \operatorname{Exp}(\Delta \models p \land \Theta);$
- (6)  $\operatorname{Exp}(\Delta \models \mathcal{F}(\Psi)) = \operatorname{Exp}(\mathcal{F}^{\dagger}(\Delta) \models \Psi)$  for any  $\Psi \in \mathcal{A}_{W'}$  and any completely positive and sub-unital super-operator  $\mathcal{F}$  from  $\mathcal{H}_{W'}$  to  $\mathcal{H}_W$ .

### ▶ Lemma 22 (Lemma 3.10, [16]).

- (1) For any cq-states  $\Delta$  and  $\Delta'$  in  $S_V$ ,
  - if  $\Delta \sqsubseteq \Delta'$ , then  $\operatorname{Exp}(\Delta \models \Theta) \leq \operatorname{Exp}(\Delta' \models \Theta)$  for all  $\Theta \in \mathcal{A}_W$  with  $W \subseteq V$ ;
  - $= \text{ conversely, if } \operatorname{Exp}(\Delta \models \Theta) \leq \operatorname{Exp}(\Delta' \models \Theta) \text{ for all } \Theta \in \mathcal{A}_V \text{, then } \Delta \sqsubseteq \Delta'.$
- (2) For any cq-assertions  $\Theta$  and  $\Theta'$  with  $W = qv(\Theta) \cup qv(\Theta')$ ,
  - = if  $\Theta \lesssim \Theta'$ , then  $\operatorname{Exp}(\Delta \models \Theta) \leq \operatorname{Exp}(\Delta \models \Theta')$  for all  $\Delta \in \mathcal{S}_V$  with  $W \subseteq V$ ;
  - = conversely, if  $\operatorname{Exp}(\Delta \models \Theta) \leq \operatorname{Exp}(\Delta \models \Theta')$  for all  $\Delta \in \mathcal{S}_W$ , then  $\Theta \lesssim \Theta'$ .

▶ Lemma 23 (Lemma 3.11, [16]). For any cq-states  $\Delta, \Delta_n \in S_V$  and cq-assertions  $\Theta, \Theta_n \in A_W$  with  $W \subseteq V$ ,  $n = 1, 2, \cdots$ ,

- (1)  $\operatorname{Exp}(\bigvee_{n\geq 0} \Delta_n \models \Theta) = \sup_{n\geq 0} \operatorname{Exp}(\Delta_n \models \Theta)$  for increasing sequence  $\{\Delta_n\}_n$ ;
- (2)  $\operatorname{Exp}(\bigwedge_{n\geq 0} \Delta_n \models \Theta) = \inf_{n\geq 0} \operatorname{Exp}(\Delta_n \models \Theta)$  for decreasing sequence  $\{\Delta_n\}_n$ ;
- (3)  $\operatorname{Exp}(\Delta \models \bigvee_{n>0} \Theta_n) = \sup_{n\geq 0} \operatorname{Exp}(\Delta \models \Theta_n)$  for increasing sequence  $\{\Theta_n\}_n$ ;
- (4)  $\operatorname{Exp}(\Delta \models \bigwedge_{n \ge 0} \Theta_n) = \inf_{n \ge 0} \operatorname{Exp}(\Delta \models \Theta_n)$  for decreasing sequence  $\{\Theta_n\}_n$ .

The following lemma presents the explicit form for denotational semantics of various constructs for sequential programs, which extends [16, Lemma 4.6].

▶ Lemma 24. For any cq-states  $\langle \sigma, \rho \rangle$  and  $\Delta$  in  $S_V$  where V contains all quantum variables of the corresponding program,

- (1)  $[[skip]](\Delta) = \Delta$ ,  $[[abort]](\Delta) = \bot_V$ ;
- (2)  $\llbracket x := e \rrbracket(\sigma, \rho) = \langle \sigma[\sigma(e)/x], \rho \rangle;$

(3)  $\llbracket x :=_{\$} g \rrbracket(\sigma, \rho) = \sum_{d \in D_{tune(x)}} \langle \sigma[d/x], g(d) \cdot \rho \rangle;$ 

- (4)  $[[x := \mathbf{meas} \ \mathcal{M}[\bar{q}]]](\sigma, \rho) = \sum_{i \in I} \langle \sigma[i/x], M_i \rho M_i^{\dagger} \rangle$  where  $M_i$ 's are applied on  $\bar{q}$ , and  $\mathcal{M} = \{M_i : i \in I\}$ ;
- (5)  $\llbracket q := 0 \rrbracket (\sigma, \rho) = \langle \sigma, \sum_{i=0}^{d_q-1} | 0 \rangle_q \langle i | \rho | i \rangle_q \langle 0 | \rangle \rangle;$
- (6)  $\llbracket \bar{q} *= U \rrbracket (\sigma, \rho) = \langle \sigma, U_{\bar{q}} \rho U_{\bar{q}}^{\dagger} \rangle.$
- (7)  $[[S_0; S_1]](\Delta) = [[S_1]]([[S_0]](\Delta));$
- (8)  $\llbracket \mathbf{if} \square_{i=1}^{n} B_i \to S_i \mathbf{fi} \rrbracket(\Delta) = \sum_{i=1}^{n} \llbracket S_i \rrbracket(\Delta|_{B_i});$

(9)  $\llbracket \operatorname{do} \Box_{i=1}^{n} B_{i} \to S_{i} \operatorname{od} \rrbracket(\Delta) = \bigvee_{k} \llbracket S^{k} \rrbracket(\Delta), \text{ where } S \triangleq \operatorname{do} \Box_{i=1}^{n} B_{i} \to S_{i} \operatorname{od}, S^{0} \triangleq \operatorname{abort},$ and for any  $k \ge 0$ ,

$$S^{k+1} \triangleq \mathbf{if} \square_{i=1}^n B_i \to S_i; S^k \square B_0 \to \mathbf{skip} \mathbf{fi}.$$

*Here* 
$$B_0 \triangleq \bigwedge_{i=1}^n \neg B_i$$
. *Thus*  $[[S]](\Delta) = \Delta|_{B_0} + \sum_{i=1}^n [[S]]([[S_i]](\Delta|_{B_i}))$ .

**Proof.** Similar to that of [16, Lemma 4.6].

# C Omitted proofs

**Proof of Lemma 6.** Induction on the structure of S.

**Proof of Lemma 7.** This can be easily seen from the fact that the only successor configuration of a terminal one under  $\rightarrow$  is itself.

# C.1 Proof of Theorem 9

To prove Theorem 9, we first introduce some notions. Note that from Table 1, any transition  $\langle S, \sigma, \rho \rangle \rightarrow \mu$  of a distributed program S must be obtained by using (Paral) or (Comm). To make it clear which processes are involved in the transition, we write  $\langle S, \sigma, \rho \rangle \xrightarrow{k} \mu$  if it is caused by a local action of process  $S_k$ . Similarly, we write  $\langle S, \sigma, \rho \rangle \xrightarrow{(k,\ell)} \mu$  if it is caused by a communication between processes  $S_k$  and  $S_\ell$  with  $k < \ell$ . Let  $\mathcal{T} \triangleq [n] \cup \{(k,\ell) \in [n]^2 : k < \ell\}$ , where  $[n] \triangleq \{1, \ldots, n\}$ , be the set of possible transition labels.

▶ **Definition 25.** Let  $\pi = {\mu_i : i \ge 0}$  be a computation of  $\langle S, \sigma, \rho \rangle$ . The (infinite) *derivative tree T* induced by  $\pi$  is defined as follows: for all  $i \ge 0$ ,

- (1) nodes at the *i*-th level of T are support configurations of  $\mu_i$ . In particular, the root node of T is  $\langle S, \sigma, \rho \rangle$ ;
- (2) for any *i*-th level node c (thus c ∈ [µ<sub>i</sub>]) which is not a terminal, if c A → ν, A ∈ T, is the transition from c which contributes to the evolvement from µ<sub>i</sub> to µ<sub>i+1</sub>, then there is an edge in T from c to each support configuration of ν. Furthermore, these edges are labelled by action A and their corresponding probabilities in ν;
- (3) for any terminal configuration c at the *i*-th level, note that c also appears at the i + 1-th level. Then there is an edge in T from the *i*-th level c to the i + 1-th level c. Furthermore, this edge is labelled by a special symbol \* and probability 1.

Note that from a derivative tree T, we can easily recover the computation  $\{\mu_i : i \ge 0\}$  as follows: for each  $i \ge 0$ , let  $N_i$  be the set of nodes at the *i*-th level of T. Then

$$\mu_i = \sum_{c \in N_i} p_c \cdot c$$

where  $p_c$  is the product of all the probabilities along the path from the root to c.

**Definition 26.** Let  $\pi$  be a computation of  $\langle S, \sigma, \rho \rangle$ , and T its derivative tree.

- (1) A run  $r = \{c_i : i \ge 0\}$  of  $\pi$  is a path of T starting from the root node (thus  $c_0 = \langle S, \sigma, \rho \rangle$ ).
- (2) The history of a run r = {c<sub>i</sub> : i ≥ 0} is a sequence {(E<sub>i</sub>, A<sub>i</sub>) ∈ 2<sup>T</sup> × (T ∪ {\*}) : i ≥ 0} such that E<sub>i</sub> is the set of transition labels that are enabled in c<sub>i</sub>, while A<sub>i</sub> is the label on the edge (c<sub>i</sub>, c<sub>i+1</sub>) in T. Note that A<sub>i</sub> ∈ E<sub>i</sub> whenever E<sub>i</sub> ≠ Ø.

Fix arbitrarily a linear order  $\sqsubseteq$  over  $\mathcal{T}$ . For example, we may let  $A \sqsubseteq B$  if (1)  $A \in [n]$  and  $B \in [n]^2$ , or (2) A < B when both A and B are in [n], or (3) i < j when A = (i, k) and  $B = (j, \ell)$ .

-

▶ **Definition 27.** A run is good if its history  $\{(E_i, A_i) : i \ge 0\}$  satisfies the following condition:

$$\forall i \ge 0 : (E_i \neq \emptyset \to A_i = \min E_i)$$

where min  $E_i$  is the minimum element in  $E_i$  according to the linear order  $\sqsubseteq$ . A computation  $\pi$  is good if all of its runs are good.

We are now ready to prove the main theorem of this section, which says that all computations from a given input computes the same cq-state.

**Proof of Theorem 9.** Note that from any configuration  $\langle S, \sigma, \rho \rangle$ , there exists a unique good computation. The main idea of the proof is that we can always transform the derivative tree T of any computation into that of the good one starting from the same configuration, using some 'commutativity' properties of transitions from different processes. Furthermore, this transformation does not change the computed cq-state.

Let  $\pi = {\mu_i : i \ge 0}$  be a computation with  $\mu_0 = \langle S, \sigma, \rho \rangle \xrightarrow{A} \mu_1$ , and T its derivative tree. Suppose the good computation from  $\langle S, \sigma, \rho \rangle$  would choose  $B, B \ne A$ , as the first action. We show in the following how to transform  $\pi$  into another (not necessarily good) computation  $\pi'$  with the first action being B, and they compute the same cq-state. To simplify the presentation, we assume B = kfor some  $k \in [n]$  (the case when  $B \in [n]^2$  is similar).

First, we prove that the *B*-transition must appear along every terminating run of  $\pi$ . To see this, suppose on the contrary there is a successful run r in which no *B*-transition is executed. Note that any transition which does not involve k cannot change the value of variables in  $cv(S_k)$ , and since  $S_k$  is deterministic, at most one of the actions in  $\mathcal{T}$  which involve k is enabled at any moment. Consequently, *B* will be continuously enabled along r, which is a contradiction since the quantum program in the last configuration of r must be *E*.

Now for any terminating run  $r = \{c_i : i \ge 0\}$  of  $\pi$  (thus  $c_0 = \langle S, \sigma, \rho \rangle$ ) with history  $\{(E_i, A_i) : i \ge 0\}$ , let  $c_{i_B} \triangleq \langle R_{i_B}, \sigma_{i_B}, \rho_{i_B} \rangle$  be the first configuration in which *B* is executed; that is,  $A_{i_B} = B$ , and  $A_i \ne B$  for all  $i < i_B$ . From transition rule (Paral) in Table 1 and Lemma 6, let

$$\langle S, \sigma, \rho \rangle \xrightarrow{B} \sum_{j \in J} p_j \cdot \langle R_j, f_j(\sigma), \mathcal{E}_j(\rho) / p_j \rangle$$
 (3)

where  $R_j = S_1 \| \dots \| S_{k,j} \| \dots \| S_n$  for some  $S_{k,j}$ ,  $f_j$  only depends on  $cv(S_k)$  but does not change the variables outside  $change(S_k)$ ,  $\mathcal{E}_j$  is a super-operator acting on  $\mathcal{H}_{qv(S_k)}$ , and  $p_j = tr(\mathcal{E}_j(\rho))$ . Then from the fact that along the path  $c_0, c_1, \dots, c_{i_B}$ , no action involving k is performed, the transition that happens at  $c_{i_B}$  in the computation  $\pi$  has the form

$$\langle R_{i_B}, \sigma_{i_B}, \rho_{i_B} \rangle \xrightarrow{B} \sum_{j \in J} p_{i_B,j} \cdot \langle R_{i_B,j}, f_j(\sigma_{i_B}), \mathcal{E}_j(\rho_{i_B})/p_{i_B,j} \rangle$$
 (4)

where  $R_{i_B,j} = S_1^{i_B} \| \dots \| S_{k,j} \| \dots \| S_n^{i_B}$  whenever  $R_{i_B} = S_1^{i_B} \| \dots \| S_k \| \dots \| S_n^{i_B}$ , and  $p_{i_B,j} = \operatorname{tr}(\mathcal{E}_j(\rho_{i_B}))$ .

For any  $j \in J$ , we are going to construct from T a derivative tree  $T_j$  where the first execution of the *B*-transition along any terminating run of T is replaced by the corresponding *j*-th child in the *B*-transition; that is,  $c_{i_B}$  is replaced by  $\langle R_{i_B,j}, f_j(\sigma_{i_B}), \mathcal{E}_j(\rho_{i_B})/p_{i_B,j} \rangle$ . To be more specific,  $T_j$  is constructed as follows.

- (1) Let the root of  $T_j$  be  $\langle R_j, f_j(\sigma), \mathcal{E}_j(\rho)/p_j \rangle$ .
- (2) To unfold  $T_j$  from the root, we follow precisely the transitions taken by T along each run r until the configuration  $c_{i_B}$  is reached. For such a finite path  $c_0, c_1, \ldots, c_{i_B}$  in T, it is easy to see that the corresponding path in  $T_j$  is  $c'_0, c'_1, \ldots, c'_{i_B}$ , where

$$c_i' \triangleq \langle S_1^i \| \dots \| S_{k,j} \| \dots \| S_n^i, f_j(\sigma_i), \mathcal{E}_j(\rho_i) / \operatorname{tr}(\mathcal{E}_j(\rho_i)) \rangle$$

whenever

$$c_i = \langle S_1^i \| \dots \| S_k \| \dots \| S_n^i, \sigma_i, \rho_i \rangle$$

Here in each  $c_i$  the k-th process must be  $S_k$  since along the path  $c_0, c_1, \ldots, c_{i_B}$  in T, no B-transition is executed. In particular,  $c'_{i_B}$  is precisely the j-th support configuration of the right-hand side distribution in Eq. (4). Furthermore, it is easy to check that each pair of the corresponding edges in T and  $T_j$  along each run up to the respective  $c_{i_B}$  are labelled with the same probability.

(3) The subtree of  $T_j$  rooted at  $c'_{i_B}$  is the same as the subtree of T rooted at  $c'_{i_B}$  (from the above clause,  $c'_{i_B}$  indeed appears in T as a child node of  $c_{i_B}$ ).

Finally, let T' be a derivative tree where the root is  $\langle S, \sigma, \rho \rangle$ , the action executed by the root is given in Eq. (3), and for each  $j \in J$ ,  $T_j$  is the subtree starting from  $\langle R_j, f_j(\sigma), \mathcal{E}_j(\rho)/p_j \rangle$ . Note also that the above procedure transforms non-terminating runs to non-terminating runs. Thus obviously, the induced computation  $\pi' = \{\mu'_i : i \geq 0\}$  computes the same cq-state as  $\pi$ .

Repeat the above procedure, we will eventually transform any computation to the good one without changing the cq-state computed. That concludes the proof of the theorem.

# C.2 Proof of Lemma 11

Clause (2) is easy. For (1), let  $\Delta = \langle \sigma, \rho \rangle$  with  $\operatorname{tr}(\rho) = 1$ , and  $\pi \triangleq \{\mu_i : i \ge 0\}$  a computation of S starting in  $\Delta$ . We prove by induction on i that  $\Delta_{\mu_i}$  has countable support and  $\operatorname{tr}(\Delta_{\mu_i}) \le \operatorname{tr}(\rho)$ . Thus the result holds for simple cq-states. The general case follows easily.

# C.3 Proof of Theorem 12

We first show a close relationship between the *good* transitions of S and the transitions of T(S).

**Lemma 28.** For any configuration  $(S, \sigma, \rho)$  where S is a distributed quantum program,

- (1) if the transition  $\langle S, \sigma, \rho \rangle \to \sum_{i \in I} p_i \cdot \langle S_i, \sigma_i, \rho_i \rangle$  appears in the derivative tree of a good computation, then  $\langle T(S), \sigma, \rho \rangle \to \sum_{i \in I} p_i \cdot \langle T(S_i), \sigma_i, \rho_i \rangle$  is the (unique) transition from  $\langle T(S), \sigma, \rho \rangle$ ;
- (2) conversely, if  $\langle T(S), \sigma, \rho \rangle \rightarrow \sum_{i \in I} p_i \cdot \langle S'_i, \sigma_i, \rho_i \rangle$  then either  $\langle S, \sigma, \rho \rangle \rightarrow \sum_{i \in I} p_i \cdot \langle S_i, \sigma_i, \rho_i \rangle$ appears in the derivative tree of a good computation and  $S'_i = T(S_i)$ , or  $\langle S, \sigma, \rho \rangle$  is a deadlock. In the latter case,  $\sigma \models BLOCK \land \neg TERM$ .

**Proof.** Easy from the definitions of T(S), which is a deterministic quantum program, and the good computation of S. Furthermore, if  $\langle S, \sigma, \rho \rangle$  is a deadlock, then the classical state  $\sigma$  must satisfy  $BLOCK \land \neg TERM$ .

With this lemma, Theorem 12 can be proved as follows.

**Proof of Theorem 12.** We need only prove the theorem for the case when  $\Delta = \langle \sigma, \rho \rangle$  with  $\operatorname{tr}(\rho) = 1$ . Let  $\pi \triangleq \{\mu_i : i \ge 0\}$  and  $\pi' \triangleq \{\mu'_i : i \ge 0\}$  be the computation of T(S) and the good computation of S, both starting in  $\langle \sigma, \rho \rangle$ , respectively. We are going to show that for any  $i \ge 0$ ,  $\Delta_{\mu_i} = \Delta_{\mu'_i}|_{TERM}$ . Then the theorem follows by taking the least upper bounds of both sides.

From Lemma 28, the derivative tree of  $\pi$  has the same structure (including the probability weights along the edges) with that of  $\pi'$ , except for deadlock configurations. However, Lemma 28 also says that classical states in these deadlock configurations must satisfy  $BLOCK \wedge \neg TERM$ , and thus they will be excluded in computing  $\Delta_{\mu'_i}|_{TERM}$ . Note further that TERM is satisfied by all the successfully terminating configurations in  $\mu_i$ ; that is,  $\Delta_{\mu_i} = \Delta_{\mu_i}|_{TERM}$ . Thus  $\Delta_{\mu_i} = \Delta_{\mu'_i}|_{TERM}$  as desired.

$$\begin{split} xp.\mathbf{skip}.\Theta &= \Theta \qquad wlp.\mathbf{abort}.\Theta = \top_V \qquad wp.\mathbf{abort}.\Theta = \bot_V \\ xp.(x := e).\Theta &= \Theta[e/x] \qquad xp.(x :=_{\$} g).\Theta = \sum_{d \in D_{type(x)}} g(d) \cdot \Theta[d/x] \\ xp.(\bar{q} *= U).\Theta &= U_{\bar{q}}^{\dagger}\Theta U_{\bar{q}} \qquad xp.(q := 0).\Theta = \sum_{i=0}^{d_q-1} |i\rangle_q \langle 0|\Theta|0\rangle_q \langle i| \\ xp.(S_0; S_1).\Theta &= xp.S_0.(xp.S_1.\Theta) \qquad xp.(x := \mathbf{meas} \ \mathcal{M}[\bar{q}]).\Theta &= \sum_{i \in I} M_i^{\dagger}\Theta[i/x]M_i \\ wlp.(\mathbf{if} \ \Box_{i=1}^n B_i \to S_i \ \mathbf{fi}).\Theta &= \sum_{i=1}^n B_i \wedge wlp.S_i.\Theta + \bigwedge_{i=1}^n \neg B_i \\ wp.(\mathbf{if} \ \Box_{i=1}^n B_i \to S_i \ \mathbf{fi}).\Theta &= \sum_{i=1}^n B_i \wedge wp.S_i.\Theta \\ wlp.(\mathbf{do} \ \Box_{i=1}^n B_i \to S_i \ \mathbf{od}).\Theta &= \bigwedge_{k \geq 0} \Theta_k, \text{ where } \Theta_0 \triangleq \top_V, \text{ and for any } k \geq 0, \end{split}$$

 $\Theta_{k+1} \triangleq \sum_{i=1}^{n} B_i \wedge wlp.S_i.\Theta_k + \bigwedge_{i=1}^{n} \neg B_i \wedge \Theta.$ 

 $wp.(\mathbf{do} \Box_{i=1}^{n} B_i \to S_i \mathbf{od}).\Theta = \bigvee_{k>0} \Theta_k$ , where  $\Theta_0 \triangleq \bot_V$ , and for any  $k \ge 0$ ,

$$\Theta_{k+1} \triangleq \sum_{i=1}^{n} B_i \wedge wp.S_i.\Theta_k + \bigwedge_{i=1}^{n} \neg B_i \wedge \Theta.$$

**Table 4** Weakest (liberal) precondition semantics for sequential programs, where  $xp \in \{wp, wlp\}$  and  $V = qv(\Theta)$ .

# C.4 Proof of Theorems 18 and 20

The basic idea of proving the soundness and completeness of our proof systems is to employ weakest (liberal) preconditions. To this end, we extend the weakest (liberal) precondition semantics presented in [16] to sequential programs defined in Sec. 2.1. Note that we do not have to extend it further to distributed programs, thanks to the sequentialisation theorem (Theorem 12). Let  $\mathcal{A}_{\supseteq qv(S)} \triangleq \bigcup_{V \supseteq qv(S)} \mathcal{A}_V$ .

**Definition 29.** Let S be a sequential quantum program. The weakest precondition semantics wp.S and weakest liberal precondition semantics wlp.S of S are both mappings

$$\mathcal{A}_{\supseteq qv(S)} \to \mathcal{A}_{\supseteq qv(S)}$$

defined inductively in Table 4. To simplify notation, we use xp to denote both wp and wlp whenever it is applicable for both of them.

The following lemma shows a duality relation between the denotational and weakest (liberal) precondition semantics of sequential programs, which extends [16, Lemma 4.14].

▶ **Lemma 30.** Let *S* be a sequential quantum program,  $\Delta$  a cq-state, and  $\Theta$  a cq-assertion with  $qv(\Delta) \supseteq qv(\Theta) \supseteq qv(S)$ . Then

(1)  $qv(wp.S.\Theta) = qv(wlp.S.\Theta) = qv(\Theta);$ 

(2)  $\operatorname{Exp}(\Delta \models wp.S.\Theta) = \operatorname{Exp}(\llbracket S \rrbracket(\Delta) \models \Theta);$ 

(3)  $\operatorname{Exp}(\Delta \models wlp.S.\Theta) = \operatorname{Exp}(\llbracket S \rrbracket(\Delta) \models \Theta) + \operatorname{tr}(\Delta) - \operatorname{tr}(\llbracket S \rrbracket(\Delta)).$ 

**Proof.** We prove this lemma by induction on the structure of S. The basis cases are easy from the definition. We only show the following cases for clause (3) as examples. Let  $V \triangleq qv(\Theta)$ .

• Let  $S \triangleq \mathbf{if} \square_{i=1}^{n} B_i \to S_i \mathbf{fi}$ . Note that  $B_i$ 's are mutually exclusive. Then

$$\begin{aligned} \operatorname{Exp}(\Delta \models wlp.S.\Theta) &= \operatorname{Exp}\left(\Delta \models \sum_{i=1}^{n} B_{i} \wedge wlp.S_{i}.\Theta + \bigwedge_{i=1}^{n} \neg B_{i}\right) \\ &= \sum_{i=1}^{n} \operatorname{Exp}(\Delta|_{B_{i}} \models wlp.S_{i}.\Theta) + \operatorname{Exp}\left(\Delta \models \top_{V} - \sum_{i=1}^{n} B_{i}\right) \\ &= \sum_{i=1}^{n} \left[\operatorname{Exp}\left([\![S_{i}]\!](\Delta|_{B_{i}}) \models \Theta\right) + \operatorname{tr}(\Delta|_{B_{i}}) - \operatorname{tr}([\![S_{i}]\!](\Delta|_{B_{i}}))] \right] \\ &+ \operatorname{tr}(\Delta) - \sum_{i=1}^{n} \operatorname{tr}(\Delta|_{B_{i}}) \\ &= \operatorname{Exp}([\![S]\!](\Delta) \models \Theta) + \operatorname{tr}(\Delta) - \operatorname{tr}([\![S]\!](\Delta)). \end{aligned}$$

Here the second equality follows from Lemma 21, the third one from the inductive hypothesis, and the last one from Lemma 24.

■ Let  $S \triangleq \mathbf{do} \square_{i=1}^{n} B_i \to S_i$  od and  $\Theta_k, k \ge 0$ , be defined as in Table 4 for the *wlp* semantics of  $\mathbf{do} \square_{i=1}^{n} B_i \to S_i$  od. First, we show by induction that for any  $k \ge 0$  and  $\Delta' \in \mathcal{S}_V$ ,

$$\operatorname{Exp}(\Delta' \models \Theta_k) = \operatorname{Exp}(\llbracket S^k \rrbracket(\Delta') \models \Theta) + \operatorname{tr}(\Delta') - \operatorname{tr}(\llbracket S^k \rrbracket(\Delta'))$$
(5)

where  $S^k$  is defined as in Lemma 24. The case of k = 0 follows from the definition. Let  $B \triangleq \bigwedge_{i=1}^n \neg B_i$ . We further calculate from Lemmas 21 and 24 that

$$\begin{split} &\operatorname{Exp}(\Delta' \models \Theta_{k+1}) \\ &= \operatorname{Exp}(\Delta' \models \sum_{i=1}^{n} B_{i} \wedge wlp.S_{i}.\Theta_{k}) + \operatorname{Exp}(\Delta' \models B \wedge \Theta) \\ &= \sum_{i=1}^{n} \operatorname{Exp}(\Delta'|_{B_{i}} \models wlp.S_{i}.\Theta_{k}) + \operatorname{Exp}(\Delta'|_{B} \models \Theta) \\ &= \sum_{i=1}^{n} \left[ \operatorname{Exp}\left( \mathbb{I}S_{i} \mathbb{I}(\Delta'|_{B_{i}}) \models \Theta_{k} \right) + \operatorname{tr}(\Delta'|_{B_{i}}) - \operatorname{tr}(\mathbb{I}S_{i} \mathbb{I}(\Delta'|_{B_{i}})) \right] + \operatorname{Exp}(\Delta'|_{B} \models \Theta) \\ &= \sum_{i=1}^{n} \left[ \operatorname{Exp}(\mathbb{I}S^{k} \mathbb{I}(\mathbb{I}S_{i} \mathbb{I}(\Delta'|_{B_{i}})) \models \Theta) + \operatorname{tr}(\mathbb{I}S_{i} \mathbb{I}(\Delta'|_{B_{i}})) - \operatorname{tr}(\mathbb{I}S^{k} \mathbb{I}(\mathbb{I}S_{i} \mathbb{I}(\Delta'|_{B_{i}}))) \right] \\ &\quad + \sum_{i=1}^{n} \left[ \operatorname{tr}(\Delta'|_{B_{i}}) - \operatorname{tr}(\mathbb{I}S_{i} \mathbb{I}(\Delta'|_{B_{i}})) \right] + \operatorname{Exp}(\Delta'|_{B} \models \Theta) \\ &= \operatorname{Exp}(\mathbb{I}S^{k+1} \mathbb{I}(\Delta') \models \Theta) + \operatorname{tr}(\Delta') - \operatorname{tr}(\mathbb{I}S^{k+1} \mathbb{I}(\Delta')), \end{split}$$

where the fourth equality follows from the induction hypothesis, and the last one from the fact that  $[[S^{k+1}]](\Delta') = \sum_{i=1}^{n} [[S^{k}]]([[S_{i}]](\Delta'|_{B_{i}})) + \Delta'|_{B}$  and  $\operatorname{tr}(\Delta') = \sum_{i=1}^{n} \operatorname{tr}(\Delta'|_{B_{i}}) + \operatorname{tr}(\Delta'|_{B})$ . With Eq. (5), we have from Lemma 23 that

$$\operatorname{Exp}(\Delta \models wlp.S.\Theta) = \operatorname{Exp}(\Delta \models \bigwedge_{k \ge 0} \Theta_k) = \operatorname{Exp}(\llbracket S \rrbracket(\Delta) \models \Theta) + \operatorname{tr}(\Delta) - \operatorname{tr}(\llbracket S \rrbracket(\Delta)).$$

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The following two lemmas, which extend Lemmas 4.16 and 4.17 in [16], respectively, can be similarly shown for our sequential programs. The proofs are omitted here.

▶ Lemma 31. Let *S* be a sequential program,  $\Delta$  a cq-state, and  $\Theta$  a cq-assertion with  $qv(\Delta) \supseteq qv(\Theta) \supseteq qv(S)$ . Let  $xp \in \{wp, wlp\}$ . Then

- (1)  $wp.S.\Theta + wlp.S.(\top_{qv(\Theta)} \Theta) = \top_{qv(\Theta)};$
- (2) the function xp.S is monotonic; that is, for all  $\Theta_1 \sqsubseteq \Theta_2$ ,  $xp.S.\Theta_1 \sqsubseteq xp.S.\Theta_2$ ;
- (3) the function wp.S is linear; that is, for all  $\Theta_1, \Theta_2 \in \mathcal{A}_V$ ,

 $wp.S.(\lambda_1\Theta_1 + \lambda_2\Theta_2) = \lambda_1 wp.S.\Theta_1 + \lambda_2 wp.S.\Theta_2;$ 

(4) the function wlp.S is affine-linear; that is, for all  $\Theta_1, \Theta_2 \in \mathcal{A}_V$  and  $\lambda_1 + \lambda_2 = 1$ ,

 $wlp.S.(\lambda_1\Theta_1+\lambda_2\Theta_2)=\lambda_1wlp.S.\Theta_1+\lambda_2wlp.S.\Theta_2.$ 

(5) if  $W \cap qv(\Theta) \subseteq V \subseteq qv(\Theta)$ ,  $(V \cup W) \cap qv(S) = \emptyset$ , and  $\mathcal{F}_{V \to W}$  is a completely positive and sub-unital super-operator, then

$$\mathcal{F}_{V \to W}(wp.S.\Theta) = wp.S.(\mathcal{F}_{V \to W}(\Theta))$$

and

$$\mathcal{F}_{V \to W}(wlp.S.\Theta) \sqsubseteq wlp.S.(\mathcal{F}_{V \to W}(\Theta)).$$

*The equality holds for wlp as well if*  $\mathcal{F}_{V \to W}$  *is unital;* 

**Lemma 32.** Let S be a sequential program, and  $\Theta$  and  $\Psi$  are cq-assertions. Then

 $\models_{tot} \{\Theta\} \ S \ \{\Psi\} \quad iff \quad \Theta \lesssim wp.S.(\Psi \otimes I_{qv(S) \setminus qv(\Psi)})$  $\models_{par} \{\Theta\} \ S \ \{\Psi\} \quad iff \quad \Theta \lesssim wlp.S.(\Psi \otimes I_{qv(S) \setminus qv(\Psi)}).$ 

In particular, if  $qv(\Theta) = qv(\Psi) \supseteq qv(S)$ , then

 $\models_{tot} \{\Theta\} \ S \ \{\Psi\} \quad iff \quad \Theta \sqsubseteq wp.S.\Psi \\ \models_{par} \{\Theta\} \ S \ \{\Psi\} \quad iff \quad \Theta \sqsubseteq wlp.S.\Psi.$ 

The next lemma shows a closed relationship between the correctness of a distributed quantum program S and its sequentialisation T(S).

**Lemma 33.** For any distributed program S and a cq-assertions  $\Theta$  and  $\Psi$ ,

 $\models_{tot} \{\Theta\} S \{\Psi \land TERM\} iff \models_{tot} \{\Theta\} T(S) \{\Psi \land TERM\}$  $\models_{par} \{\Theta\} S \{\Psi \land TERM\} iff \models_{par} \{\Theta\} T(S) \{\Psi \land TERM + \neg TERM \land BLOCK\}.$ 

**Proof.** The first equivalence is direct from Theorem 12. For the second one, let  $\Psi' \triangleq \Psi \land TERM + \neg TERM \land BLOCK$ . It suffices to prove for any  $\Delta \in S_V$  with  $V \supseteq qv(\Psi, \Theta, S)$ ,

$$\operatorname{Exp}(\llbracket T(S) \rrbracket(\Delta) \models \Psi') - \operatorname{tr}(\llbracket T(S) \rrbracket(\Delta)) = \operatorname{Exp}(\llbracket S \rrbracket(\Delta) \models \Psi \wedge TERM) - \operatorname{tr}(\llbracket S \rrbracket(\Delta))$$
(6)

Note that all support configurations in  $[T(S)](\Delta)$  satisfy *BLOCK*. Thus

$$\llbracket T(S) \rrbracket(\Delta) = \llbracket S \rrbracket(\Delta) + \llbracket T(S) \rrbracket(\Delta) |_{\neg TERM \land BLOCK}$$

from Theorem 12, and

$$\operatorname{tr}(\llbracket T(S) \rrbracket(\Delta)) = \operatorname{tr}(\llbracket S \rrbracket(\Delta)) + \operatorname{Exp}(\llbracket T(S) \rrbracket(\Delta)) \models \neg TERM \land BLOCK).$$

Then Eq. (6) follows easily from the first equivalence.

We are now ready to prove the soundness and completeness of our proof systems.

**Proof of Theorem 18. Soundness**: We need only to show that each rule in Table 2 is valid in the sense of partial correctness. The proof is divided into two steps:

(1) We first prove by structural induction that the proof rules are sound for sequential programs (thus the rule (Dist) is no applicable). We take (Rep) as an example; the others are simpler. Let S ≜ do □<sub>i=1</sub><sup>n</sup> B<sub>i</sub> → S<sub>i</sub> od, and ⊨<sub>par</sub> {B<sub>i</sub> ∧ Θ} S<sub>i</sub> {Θ} for all 1 ≤ i ≤ n. Without loss of generality, we assume qv(S) ⊆ qv(Θ). Then B<sub>i</sub> ∧ Θ ⊑ wlp.S<sub>i</sub>.Θ from Lemma 32. We now prove by induction on k that Θ ⊑ Θ<sub>k</sub> for any k ≥ 0, where Θ<sub>k</sub> is defined as in Table 4 for the wlp semantics of do □<sub>i=1</sub><sup>n</sup> B<sub>i</sub> → S<sub>i</sub> od when the postcondition is ∧<sub>i=1</sub><sup>n</sup> ¬B<sub>i</sub> ∧ Θ. The case when k = 0 is trivial. Then we calculate

$$\Theta_{k+1} = \sum_{i=1}^{n} B_i \wedge wlp.S_i.\Theta_k + \bigwedge_{i=1}^{n} \neg B_i \wedge \Theta$$
$$\supseteq \sum_{i=1}^{n} B_i \wedge wlp.S_i.\Theta + \bigwedge_{i=1}^{n} \neg B_i \wedge \Theta$$
$$\supseteq \sum_{i=1}^{n} B_i \wedge \Theta + \bigwedge_{i=1}^{n} \neg B_i \wedge \Theta = \Theta,$$

where the first inequality follows from the induction hypothesis and Lemma 31. Thus

$$\Theta \sqsubseteq wlp.(\mathbf{do} \square_{i=1}^{n} B_{i} \to S_{i} \mathbf{od}).\left(\bigwedge_{i=1}^{n} \neg B_{i} \land \Theta\right),$$

and so

$$\models_{par} \{\Theta\} \ \mathbf{do} \ \Box_{i=1}^{n} B_{i} \to S_{i} \ \mathbf{od} \ \left\{ \bigwedge_{i=1}^{n} \neg B_{i} \land \Theta \right\}$$

by Lemma 32.

(2) For generic distributed program, the only relevant rules are (Imp) and (Dist). The former is direct from Lemma 32. For (Dist), let S ≜ S<sub>1</sub> || ... ||S<sub>n</sub> and T(S) be its sequentialisation defined in Sec. 4. Suppose |=<sub>par</sub> {Θ} S<sub>1,0</sub>; ...; S<sub>n,0</sub> {Ψ}, and for all (i, j, k, l) ∈ Γ,

 $\models_{par} \{B_{i,j} \land B_{k,\ell} \land \Psi\} \ \textit{Effect}(\alpha_{i,j}, \alpha_{k,\ell}); S_{i,j}; S_{k,\ell} \ \{\Psi\}.$ 

Note that T(S) is sequential. First, by the soundness of (Imp) for sequential programs, we have

 $\models_{par} \{B_{i,j} \land B_{k,\ell} \land B_i \land \Psi\} Effect(\alpha_{i,j}, \alpha_{k,\ell}); S_{i,j}; S_{k,\ell} \{\Psi\}.$ 

Then  $\models_{par} \{\Theta\} T(S) \{\Psi \land BLOCK\}$  by using the soundness of (Seq) and (Rep) for sequential programs. Note that  $\Psi \land BLOCK \sqsubseteq \Psi'$  where  $\Psi'$  is defined in Lemma 33. Thus from (Imp) and Lemma 33 we have  $\models_{par} \{\Theta\} S \{\Psi \land TERM\}$ .

Completeness: The proof for completeness is also divided into two steps:

(1) We first prove by induction on the structure of S that for any  $\Theta$  and sequential program S with  $qv(S) \subseteq qv(\Theta), \vdash_{par} \{wlp.S.\Theta\} S \{\Theta\}$ . We take the case for loops as an example. Let  $S \triangleq \mathbf{do} \square_{i=1}^{n} B_i \to S_i$  od and  $\Psi \triangleq wlp.S.\Theta$ . By induction, we have  $\vdash_{par} \{wlp.S_i.\Psi\} S_i \{\Psi\}$  for any  $1 \leq i \leq n$ . Note that

$$\Psi = \sum_{i=1}^{n} B_i \wedge wlp.S_i.\Psi + \bigwedge_{i=1}^{n} \neg B_i \wedge \Theta$$

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Thus  $B_i \wedge \Psi = B_i \wedge wlp.S_i.\Psi \sqsubseteq wlp.S_i.\Psi$  and so  $\vdash_{par} \{B_i \wedge \Psi\}$   $S_i \{\Psi\}$  by the (Imp) rule. Now using (Rep) we have  $\vdash_{par} \{\Psi\}$  do  $\Box_{i=1}^n B_i \to S_i$  od  $\{\bigwedge_{i=1}^n \neg B_i \wedge \Psi\}$  and the result follows from the fact that  $\bigwedge_{i=1}^n \neg B_i \wedge \Psi = \bigwedge_{i=1}^n \neg B_i \wedge \Theta \sqsubseteq \Theta$ .

(2) Let  $S \triangleq S_1 \parallel \ldots \parallel S_n$  and T(S) its sequentialisation defined in Sec. 4. Suppose  $\models_{par} \{\Theta\} S \{\Psi\}$ . Note that for any  $\Delta \in S_V$  with  $V \supseteq qv(\Psi, \Theta, S)$ , all support configurations in  $[[S]](\Delta)$  satisfy *TERM*. Thus  $\models_{par} \{\Theta\} S \{\Psi \land TERM\}$ . Then from Lemma 33, we have  $\models_{par} \{\Theta\} T(S) \{\Theta'\}$  where  $\Theta' \triangleq \Psi \land TERM + \neg TERM \land BLOCK$ , and thus  $\Theta \lesssim wlp.T(S).\Theta'$ . Let  $\Psi' \triangleq wlp.do.\Theta'$  where do is the do-loop in T(S). As T(S) is sequential, we have from the above clause that

 $\vdash_{par} \{\Psi'\} \text{ do } \{\Theta'\}$  and  $\vdash_{par} \{wlp.S_0.\Psi'\} S_0 \{\Psi'\}$ 

where  $S_0 \triangleq S_{1,0}; \ldots; S_{n,0}$ . Note that

$$\Psi' = \sum_{(i,j,k,\ell)\in\Gamma} B_{i,j} \wedge B_{k,\ell} \wedge B_i \wedge wlp.S_{i,j}^{k,\ell}.\Psi' + BLOCK \wedge \Theta'$$

where  $S_{i,j}^{k,\ell} \triangleq Effect(\alpha_{i,j}, \alpha_{k,\ell}); S_{i,j}; S_{k,\ell}$ . Thus

$$B_{i,j} \wedge B_{k,\ell} \wedge \Psi' = B_{i,j} \wedge B_{k,\ell} \wedge B_i \wedge wlp.S_{i,j}^{k,\ell}.\Psi' \sqsubseteq wlp.S_{i,j}^{k,\ell}.\Psi',$$

and so

$$\vdash_{par} \{B_{i,j} \land B_{k,\ell} \land \Psi'\} S_{i,j}^{k,\ell} \{\Psi'\}.$$

by (Imp) and the completeness result for sequential quantum programs. Note that  $wlp.S_0.\Psi' = wlp.T(S).\Theta'$ . Applying (Dist) and (Imp), we derive  $\vdash_{par} \{\Theta\} S \{\Psi' \land TERM\}$ , and the result follows from the fact that  $\Psi' \land TERM = \Theta' \land TERM = \Psi \land TERM \sqsubseteq \Psi$ .

The proof for total correctness is more involved.

**Proof of Theorem 20. Soundness**: Similar to the partial correctness case, the proof is divided into two steps:

(1) We first prove by structural induction that the proof rules in Table 2 with the corresponding rules replaced by those in Table 3 are sound for sequential programs (thus the rule (Dist-T) is no applicable), in the sense of total correctness. Again, we take (Rep-T) as an example. Let S ≜ do □<sub>i=1</sub><sup>n</sup>B<sub>i</sub> → S<sub>i</sub> od, ⊨<sub>tot</sub> {B<sub>i</sub> ∧ Θ} S<sub>i</sub> {Θ} for all 1 ≤ i ≤ n, and {Ψ<sub>k</sub> : k ≥ 0} be a sequence of Θ-ranking assertions for S. Without loss of generality, we assume qv(S) ⊆ qv(Θ). We now prove by induction on k that Θ ⊑ Θ<sub>k</sub> + Ψ<sub>k</sub> for any k ≥ 0, where Θ<sub>k</sub> is defined as in Table 4 for the wp semantics of do □<sub>i=1</sub><sup>n</sup>B<sub>i</sub> → S<sub>i</sub> od when the postcondition is Λ<sub>i=1</sub><sup>n</sup> ¬B<sub>i</sub> ∧ Θ. The case when k = 0 is from the fact that Θ ⊑ Ψ<sub>0</sub>. Then from the inductive hypothesis and Lemmas 31 and 32,

$$B_i \land \Theta \sqsubseteq wp.S_i.\Theta \sqsubseteq wp.S_i.\Theta_k + wp.S_i.\Psi_k$$

and so

$$\Theta_{k+1} + \Psi_{k+1} \supseteq \sum_{i=1}^{n} B_i \wedge wp.S_i.\Theta_k + \bigwedge_{i=1}^{n} \neg B_i \wedge \Theta + \sum_{i=1}^{n} B_i \wedge wp.S_i.\Psi_k$$
$$\supseteq \sum_{i=1}^{n} B_i \wedge \Theta + \bigwedge_{i=1}^{n} \neg B_i \wedge \Theta = \Theta,$$

4

where the first inequality follows from the definition of ranking assertions and the fact that  $B_i$ 's are mutually exclusive, and the second one from the induction hypothesis. Thus

$$\Theta \sqsubseteq wp.(\mathbf{do} \square_{i=1}^{n} B_{i} \to S_{i} \mathbf{od}).\left(\bigwedge_{i=1}^{n} \neg B_{i} \land \Theta\right)$$

by noting that  $\bigwedge_k \Psi_k = \bot_V$ , and so

$$\models_{tot} \{\Theta\} \ \mathbf{do} \ \Box_{i=1}^{n} B_{i} \to S_{i} \ \mathbf{od} \ \left\{ \bigwedge_{i=1}^{n} \neg B_{i} \land \Theta \right\}$$

as desired.

- (2) For generic distributed programs, again we only consider (Dist). The proof is similar to the case for partial correctness, by noting the following two facts: for any distributed program S and cq-assertion  $\Psi$ ,
  - ranking assertions for S are also ranking assertions for the do-loop of T(S);
  - from the assumption  $\Psi \wedge BLOCK \lesssim TERM$  we have  $\Psi \wedge BLOCK = \Psi \wedge TERM$ .

Completeness: The proof for completeness is also divided into two steps:

(1) We first prove by induction on the structure of S that for any  $\Theta$  and sequential program S with  $qv(S) \subseteq qv(\Theta), \vdash_{tot} \{wp.S.\Theta\} \ S \ \{\Theta\}$ . Again, we take the case for loops as an example. Let  $S \triangleq \mathbf{do} \square_{i=1}^{n} B_i \to S_i$  od and  $\Psi \triangleq wp.S.\Theta$ . By induction, we have  $\vdash_{tot} \{wp.S_i.\Psi\} \ S_i \ \{\Psi\}$  for any  $1 \leq i \leq n$ . Note that

$$\Psi = \sum_{i=1}^{n} B_i \wedge wp.S_i.\Psi + \bigwedge_{i=1}^{n} \neg B_i \wedge \Theta.$$

Thus  $B_i \wedge \Psi = B_i \wedge wp.S_i.\Psi \sqsubseteq wp.S_i.\Psi$  and so  $\vdash_{tot} \{B_i \wedge \Psi\} S_i \{\Psi\}$  by the (Imp) rule. Let  $\Theta_0 \triangleq wp.S.\top_{qv(\Theta)}$  and  $\Theta_{k+1} \triangleq \sum_{i=1}^n B_i \wedge wp.S_i.\Theta_k$ . We are going to show that  $\{\Theta_k : k \ge 0\}$  are  $\Psi$ -ranking assertions for S. First, note that

$$\Theta_1 = \sum_{i=1}^n B_i \wedge wp.S_i.\Theta_0 \sqsubseteq \bigwedge_{i=1}^n \neg B_i \wedge \top_{qv(\Theta)} + \sum_{i=1}^n B_i \wedge wp.S_i.\Theta_0 = \Theta_0.$$

So  $\{\Theta_k : k \ge 0\}$  is decreasing by easy induction, using Lemma 31(2). Next, as  $\Theta \sqsubseteq \top_{qv(\Theta)}$ , we have  $\Psi \sqsubseteq \Theta_0$ .

Finally, we prove that  $\bigwedge_k \Theta_k = \bot_{qv(\Theta)}$ . We show by induction on k that for any  $k \ge 0$  and  $\Delta \in S_{qv(\Theta,S)}$ ,

$$\operatorname{Exp}(\Delta \models \Theta_k) = \operatorname{tr}(\llbracket S \rrbracket(\Delta)) - \operatorname{tr}(\llbracket S^k \rrbracket(\Delta)).$$
(7)

The case when k = 0 is direct from Lemmas 21 and 30. We further calculate that

$$\begin{aligned} \operatorname{Exp}(\Delta \models \Theta_{k+1}) &= \operatorname{Exp}\left(\Delta \models \sum_{i=1}^{n} B_{i} \wedge wp.S_{i}.\Theta_{k}\right) \\ &= \sum_{i=1}^{n} \operatorname{Exp}(\Delta \mid_{B_{i}} \models wp.S_{i}.\Theta_{k}) \\ &= \sum_{i=1}^{n} \operatorname{Exp}(\llbracket S_{i} \rrbracket(\Delta \mid_{B_{i}}) \models \Theta_{k}) \\ &= \sum_{i=1}^{n} \operatorname{tr}(\llbracket S \rrbracket(\llbracket S \rrbracket(\Delta \mid_{B_{i}}))) - \sum_{i=1}^{n} \operatorname{tr}(\llbracket S^{k} \rrbracket(\llbracket S_{i} \rrbracket(\Delta \mid_{B_{i}}))) \\ &= \operatorname{tr}(\llbracket S \rrbracket(\Delta)) - \operatorname{tr}(\llbracket S^{k+1} \rrbracket(\Delta)). \end{aligned}$$

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$$\begin{array}{l} \text{(C-Rep-T)} & \frac{\{B_i \land \Theta\} \ S_i \ \{\Theta\}, \{B_i \land p \land t = z\} \ S_i \ \{t < z\}, \forall i \in \{1, \ldots, n\}, \ p \to t \ge 0}{\{\Theta\} \ \text{do } \Box_{i=1}^n B_i \to S_i \ \text{od } \{\Theta \land \bigwedge_{i=1}^n \neg B_i\}} \\ \\ \text{where } type(z) = type(t) = \textbf{Integer}, z \not\in cv(p, B_i, t, S_i), \Theta = \bigoplus_{i \in I} \langle p_i, M_i \rangle \text{ and } p \triangleq \bigvee_{i \in I} p_i. \\ \\ \{\Theta\} \ S_{1,0}; \ldots; S_{n,0} \ \{\Psi\}, \ p \to t \ge 0, \ p \land BLOCK \to TERM \\ \\ \{B_{i,j} \land B_{k,\ell} \land p \land t = z\} \ Effect(\alpha_{i,j}, \alpha_{k,\ell}); S_{i,j}; S_{k,\ell} \ \{t < z\}, \forall (i, j, k, \ell) \in \Gamma \\ \\ \\ \hline \{B_{i,j} \land B_{k,\ell} \land \Psi\} \ Effect(\alpha_{i,j}, \alpha_{k,\ell}); S_{i,j}; S_{k,\ell} \ \{\Psi\}, \forall (i, j, k, \ell) \in \Gamma \\ \\ \hline \{\Theta\} \ S_1 \| \ldots \|S_n \ \{\Psi \land TERM\} \\ \\ \text{where } \Gamma, \ TERM, \ \text{and } BLOCK \ \text{are defined as in Sec. } 4, \\ \\ type(z) = type(t) = \ \textbf{Integer}, z \notin cv(p, t, S_1 \| \ldots \|S_n), \Psi = \bigoplus_{i \in I} \langle p_i, M_i \rangle, \ \text{and } p \triangleq \bigvee_{i \in I} p_i. \end{array}$$

**Table 5** Auxiliary rules.

Here the second last equality is from induction hypothesis, and the last one from Lemma 24. Note that the second term of the r.h.s of Eq.(7) converges to the first one when k goes to infinity. Thus  $\lim_k \operatorname{Exp}(\Delta \models \Theta_k) = 0$ , and so  $\bigwedge_k \Theta_k = \bot_{qv(\Theta)}$  from the arbitrariness of  $\Delta$ . Now using (Rep-T) we have  $\vdash_{tot} \{\Psi\}$  do  $\Box_{i=1}^n B_i \to S_i$  od  $\{\bigwedge_{i=1}^n \neg B_i \land \Psi\}$  and the result follows from the fact that  $\bigwedge_{i=1}^n \neg B_i \land \Psi = \bigwedge_{i=1}^n \neg B_i \land \Theta \sqsubseteq \Theta$ .

(2) The case for generic distributed programs S is similar to that for partial correctness. The construction of ranking assertions for the **do**-loop of T(S), which also work for S, follows the same approach in the above clause.

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# **D** Auxiliary Rules

We have provided sound and relatively complete proof systems for both partial and total correctness of distributed quantum programs. Thus in principle, these proof rules are sufficient for proving desired properties as long as they can be described faithfully with Hoare triple formulas. However, in practice, using these rules directly might be complicated. To simplify reasoning, we introduce two auxiliary proof rules in Table 5 for the special case when a classical ranking function can be found to guarantee the (finite) termination of repetitive sequential (C-Rep-T) or distributed (C-Dist-T) quantum programs. More auxiliary proof rules (for deterministic quantum programs) can be found in [16, 41]. For the sake of convenience, we write  $\langle p, |\psi\rangle \rangle$  for  $\langle p, |\psi\rangle \langle \psi| \rangle$ , and p for  $p \wedge \top_V$  for some appropriate V.

▶ **Theorem 34.** The auxiliary rules presented in Table 5 are sound with respect to total correctness.

**Proof.** First note that for any  $i, \models_{tot} \{B_i \land p \land t = z\} S_i \{t < z\}$  implies for any  $\sigma \models B_i \land p \land t = z$  and  $\rho$ , and any  $\sigma'$  in the support of  $[S_i](\sigma, \rho)$ , we have  $\sigma' \models t < z$ . Then an argument similar to that for classical programs leads to the conclusion that all computations from  $\langle \mathbf{do} \square_{i=1}^n B_i \to S_i \mathbf{od}, \sigma, \rho \rangle$  terminates within  $\sigma(t)$  steps, provided  $\sigma \models p$ . That proves (C-Rep-T). The case for (C-Dist-T) is similar.

### E Case studies

To illustrate the effectiveness of the proof systems as well as the auxiliary rules presented in this paper, we employ them to verify the quantum teleportation protocol. A protocol to locally implement

nonlocal gates is also investigated.

#### E.1 Verification of quantum teleportation

► Example 35 (Correctness of Quantum Teleportation). The correctness of quantum teleportation can be stated as follows: for any  $|\psi\rangle \in \mathcal{H}_2$ ,

$$\vdash_{tot} \{ |\psi\rangle_q \otimes |\beta\rangle_{q_1,q_2} \} \ Teleport \ \{ |\psi\rangle_{q_2} \}$$
(8)

The main technique of proving Eq. (8) is to employ rule (C-Dist-T). Let  $t \triangleq 2 - stage_A$  and

$$\begin{split} \Psi &\triangleq \frac{1}{4} \sum_{i,j=0,1} \left( \left\langle stage_A = stage_B = 0 \land x_A = i \land z_A = j, |j,i\rangle_{q,q_1} \otimes X^i Z^j |\psi\rangle_{q_2} \right\rangle \\ &+ \left\langle stage_A = stage_B = 1 \land x_A = i \land z_A = j, |j,i\rangle_{q,q_1} \otimes Z^j |\psi\rangle_{q_2} \right\rangle \\ &+ \left\langle stage_A = stage_B = 2 \land x_A = i \land z_A = j, |j,i\rangle_{q,q_1} \otimes |\psi\rangle_{q_2} \right\rangle ). \end{split}$$

The proof consists of three parts.

(1) We show that  $\Psi$  is a global invariant for the distributed programs *Teleport*. To this end, consider the first branch of the do-loop in T(Telepor) presented in Example 13:

$$\left\{ stage_A = stage_B = 0 \land \Psi \right\}$$

$$\left\{ \frac{1}{4} \sum_{i,j=0,1} \left\langle x_A = i \land z_A = j, |j,i\rangle_{q,q_1} \otimes X^i Z^j |\psi\rangle_{q_2} \right\rangle \right\}$$
(Imp)

 $x_B := x_A;$ 

$$\left\{\frac{1}{4}\sum_{i,j,k=0,1} \left\langle x_A = i \wedge z_A = j \wedge x_B = k, |j,i\rangle_{q,q_1} \otimes X^k Z^j |\psi\rangle_{q_2} \right\rangle\right\}$$
(Assn)

 $stage_A := 1;$ 

1

$$\left\{\frac{1}{4}\sum_{i,j,k=0,1}\left\langle stage_{A}=1\wedge x_{A}=i\wedge z_{A}=j\wedge x_{B}=k, |j,i\rangle_{q,q_{1}}\otimes X^{k}Z^{j}|\psi\rangle_{q_{2}}\right\rangle\right\} \quad (Assn)$$

 $stage_B := 1;$ 

$$\begin{cases} \sum_{k=0,1} (x_B = k) \land \mathcal{X}_{q_2}^k(\Psi) \end{cases}$$
(Assn)  
if  $x_B = 1 \rightarrow q_2 *= X \square \neg (x_B = 1) \rightarrow \text{skip fi}$   
 $\{\Psi\}$ 
(Alt)

where  $\mathcal{X}$  is the Pauli-X super-operator. Similarly, for the second branch, we can prove that

$$\{stage_A = stage_B = 1 \land \Psi \}$$
  

$$z_B := z_A; \ stage_A := 2; \ stage_B := 2; \ \mathbf{if} \ z_B = 1 \rightarrow \ q_2 \ast = Z \square \neg (z_B = 1) \rightarrow \mathbf{skip} \ \mathbf{fi}$$
  

$$\{\Psi\}.$$

(2) We show that t is a classical ranking function for the distributed program *Teleport*. Note that  $BLOCK \equiv \bigwedge_{k=0,1} \neg (stage_A = stage_B = k),$ 

$$TERM \equiv \bigwedge_{k=0,1} \neg \left( stage_A = k \right) \land \bigwedge_{k=0,1} \neg \left( stage_B = k \right)$$

and the classical part of  $\Psi$  is  $p \triangleq \bigvee_{k=0}^{2} (stage_{A} = stage_{B} = k)$ . Then it is easy to check that  $p \to t \ge 0$  and  $p \land BLOCK \to TERM$ . Furthermore, from

$$\{stage_A = stage_B = 0 \land p \land 2 - stage_A = z\}$$

$$\{1 < z\}$$

$$\{1 < z\}$$

$$\{1 < z\}$$

$$\{1 < z\}$$

$$(Imp)$$

$$stage_A := 1;$$

$$\{2 - stage_A < z\}$$

$$(Assn)$$

$$stage_B := 1;$$

$$if \ x_B = 1 \rightarrow \ q_2 *= X \square \neg (x_B = 1) \rightarrow$$

$$skip \ fi$$

$$\{2 - stage_A < z\}$$

$$(Assn, Alt)$$

and similarly for the second branch of the **do**-loop, the integer expression t is indeed a classical ranking function for *Teleport*.

(3) We show that the sequential part of T(Teleport) establishes  $\Psi$  from the precondition  $|\psi\rangle_q \otimes |\beta\rangle_{q_1,q_2}$ . Let  $|\psi\rangle = x|0\rangle + y|1\rangle$  for some  $x, y \in \mathbb{C}$ . Then

$$\begin{split} \{|\psi\rangle_q \otimes |\beta\rangle_{q_1,q_2} \} \\ q, q_1 &= CNOT; \\ \left\{ \frac{1}{\sqrt{2}} \left( x|0\rangle_q (|00\rangle + 11\rangle)_{q_1,q_2} + y|1\rangle_q (|10\rangle + 01\rangle)_{q_1,q_2} \right) \right\} \\ q &= H; \end{split} \tag{Unit}$$

$$\left\{\frac{1}{2}\left(x(|0\rangle+|1\rangle)_{q}(|00\rangle+11\rangle)_{q_{1},q_{2}}+y(|0\rangle-|1\rangle)_{q}(|10\rangle+01\rangle)_{q_{1},q_{2}}\right)\right\}$$
(Unit)

$$\left\{\sum_{i,j=0,1}\frac{1}{2}|j,i\rangle_{q,q_1}\otimes X^iZ^j|\psi\rangle_{q_2} \equiv \frac{1}{4}\sum_{i,j=0,1}\left\langle \mathbf{true},|j,i\rangle_{q,q_1}\otimes X^iZ^j|\psi\rangle_{q_2}\right\rangle\right\}$$
(*Imp*)

 $z_A := \mathbf{meas} \ q; \ x_A := \mathbf{meas} \ q_1;$ 

$$\left\{\frac{1}{4}\sum_{i,j=0,1} \langle x_A = i \wedge z_A = j, |j,i\rangle_{q,q_1} \otimes X^i Z^j |\psi\rangle_{q_2} \rangle\right\}$$
(Meas)

 $stage_A := 0; \ stage_B := 0;$ { $\Psi$ }

$$\{Assn\}$$

With the three parts shown above, we have from (C-Dist-T) that

$$\vdash_{tot} \{ |\psi\rangle_q \otimes |\beta\rangle_{q_1,q_2} \} \ Teleport \ \{ \Psi \land TERM \}$$

Then the desired result in Eq. (8) is obtained by noting that

$$\Psi \wedge TERM \equiv \frac{1}{4} \sum_{i,j=0,1} \langle stage_A = stage_B = 2 \wedge x_A = i \wedge z_A = j, |j,i\rangle_{q,q_1} \otimes |\psi\rangle_{q_2} \rangle$$

which is upper bounded above by  $|\psi\rangle_{q_2}$  according to the order  $\leq$ .

# E.2 Local implementation of nonlocal quantum gates

In distributed quantum computing, one of the key tasks is to implement quantum gates between qubits that are located in different quantum computers. To illustrate the basic idea, we recall the protocol



**Figure 2** Local implementation of remote CNOT gate. The wires from top to bottom represent qubits q,  $q_1$ ,  $q_2$ , and r respectively. Furthermore, q and  $q_1$  belong to Alice while  $q_2$  and r belong to Bob.

proposed in [12] which implements a nonlocal CNOT gate between two parties, say Alice and Bob, by employing only local quantum operations and classical communication, again with the help of a pre-shared entangled state. The protocol is depicted as in Fig. 2 and can be written as a distributed program  $RCNOT \triangleq Alice \parallel Bob$  where  $Alice \triangleq$ 

$$q, q_1 *= CNOT; x_A := \mathbf{meas} \ q_1; \ stage_A := 0;$$
  
 $\mathbf{do} \ stage_A = 0; \ c!x_A \to stage_A := 1$   
 $\Box \ stage_A = 1; \ d?z_A \to stage_A := 2; \ \mathbf{if} \ z_A = 1 \to \ q *= Z \ \Box \ \neg(z_A = 1) \to \mathbf{skip} \ \mathbf{fi}$   
 $\mathbf{od}$ 

and  $Bob \triangleq$ 

$$\begin{array}{l} q_2, r \mathrel{*=} \textit{CNOT}; \ q_2 \mathrel{*=} H; \ z_B := \mathbf{meas} \ q_2; \ stage_B := 0; \\ \mathbf{do} \ stage_B = 0; c?x_B \to stage_B := 1; \ \mathbf{if} \ x_B = 1 \to \ r \mathrel{*=} X \ \Box \ \neg(x_B = 1) \to \mathbf{skip} \ \mathbf{fi} \\ \Box \ stage_B = 1; d!z_B \to stage_B := 2 \\ \mathbf{od} \end{array}$$

The correctness of *RCNOT* is stated as follows: for any  $\alpha_{ij} \in \mathbb{C}$  with  $\sum_{i,j=0,1} |\alpha_{ij}|^2 = 1$ ,

$$\vdash_{tot} \left\{ \sum_{i,j=0,1} \alpha_{ij} | i,j \rangle_{q,r} \otimes |\beta\rangle_{q_1,q_2} \right\} RCNOT \left\{ \sum_{i,j=0,1} \alpha_{ij} | i,j \oplus i \rangle_{q,r} \right\}$$
(9)

where  $\oplus$  denotes the addition modulo 2. Again, the fact that the postcondition does not refer to  $q_1$  and  $q_2$  means that the post-measurement state of these quantum systems is irrelevant.

Similar to that of *Teleport*, to prove the correctness of *RCNOT* it suffices to show:

(1) the cq-assertion

$$\begin{split} \Psi &\triangleq \frac{1}{4} \sum_{i,j=0,1} \left( \left\langle stage_A = stage_B = 0 \land x_A = i \land z_B = j, |i,j\rangle_{q_1,q_2} \otimes X_r^i Z_q^j |\varphi\rangle_{q,r} \right\rangle \\ &+ \left\langle stage_A = stage_B = 1 \land x_A = i \land z_B = j, |i,j\rangle_{q_1,q_2} \otimes Z_q^j |\varphi\rangle_{q,r} \right\rangle \\ &+ \left\langle stage_A = stage_B = 2 \land x_A = i \land z_B = j, |i,j\rangle_{q_1,q_2} \otimes |\varphi\rangle_{q,r} \right\rangle \end{split}$$

where  $|\varphi\rangle \triangleq \sum_{k,\ell=0,1} \alpha_{k\ell} |k,\ell\rangle$ , serves as a global invariant for *RCNOT*;

(2) the expression  $t \triangleq 2 - stage_A$  is a classical ranking function; and

(3) the sequential part of *RCNOT* establishes  $\Psi$  from the precondition  $|\varphi\rangle_{q,r} \otimes |\beta\rangle_{q_1,q_2}$ . We omit the details here.