

# Quantum Programming Languages and Semantics

## 6 Denotational semantics as super-operators

This section presents a denotational (compositional) semantics for qwhile programs in the style used by CoqQ: each command denotes a *super-operator*, i.e. a linear map on operators. The key idea is that we interpret each program as a transformer of (subnormalized) density operators on the *fixed* global Hilbert space  $H \cong \bigotimes_{x \in \text{Reg}} H_x$  introduced earlier.

**Super-operators and quantum operations.** Let  $L(H)$  be the complex vector space of linear operators on  $H$ . Recall that a *super-operator* on  $H$  is a linear map  $\mathcal{E} : L(H) \rightarrow L(H)$ . Operationally, we will apply such maps to program states, i.e. to partial density operators

$$\mathcal{D}_{\leq 1}(H) := \{\rho \in L(H) : \rho \succeq 0 \wedge \text{tr}(\rho) \leq 1\}.$$

The physically meaningful state transformers are those that are *completely positive* and *trace-nonincreasing*; these are commonly called *quantum operations*. (Equivalently, they are exactly the maps admitting a Kraus form  $\mathcal{E}(\rho) = \sum_i E_i \rho E_i^\dagger$  with  $\sum_i E_i^\dagger E_i \preceq \mathbf{1}$ .) We will define denotations as super-operators and then prove that the denotations are in fact quantum operations.

We write  $\llbracket C \rrbracket$  for the denotation of a qwhile command  $C$ . Formally,  $\llbracket C \rrbracket$  is a super-operator on  $H$ :

$$\llbracket C \rrbracket : L(H) \rightarrow L(H),$$

and it restricts to a map  $\mathcal{D}_{\leq 1}(H) \rightarrow \mathcal{D}_{\leq 1}(H)$ .

A central design principle is *locality*: primitive commands mention a subsystem  $s \subseteq \text{Reg}$  and act only on  $H_s$ , leaving  $H_{\bar{s}}$  untouched. Denotationally, this is implemented using cylindrical extension.

The denotation is defined by structural recursion on the syntax of  $C$ . Here we will use the same `Cmd` as defined in the previous section, with a minor modification: we will use `abort` instead of `error`, since abnormal terminations are not our focus here.

**Skip and error.**  $\llbracket \text{skip} \rrbracket(\rho) := \rho$ ,  $\llbracket \text{abort} \rrbracket(\rho) := 0$ .

Thus `skip` is the identity super-operator, while `abort` discards all probability mass and produces no output state: once `abort` is reached, the computation does not return a normal post-state, so it contributes 0 to the overall (subnormalized) output.

**Sequencing.** Sequential composition is interpreted by function composition in the expected execution order:  $\llbracket C_1; C_2 \rrbracket := \llbracket C_2 \rrbracket \circ \llbracket C_1 \rrbracket$ , equivalently  $\llbracket C_1; C_2 \rrbracket(\rho) = \llbracket C_2 \rrbracket(\llbracket C_1 \rrbracket(\rho))$ . This clause formalizes that the output of  $C_1$  becomes the input of  $C_2$ . Because each  $\llbracket C \rrbracket$  is linear on operators,  $\llbracket C_1; C_2 \rrbracket$  is linear as well.

**Initialization.** For `init`  $\rho_s$ , recall the reset operation  $\text{Reset}_{s,\rho_s}(\rho) := \rho_s \otimes \text{tr}_s(\rho)$ . Denotationally,

$$\llbracket \text{init } \rho_s \rrbracket(\rho) := \rho_s \otimes \text{tr}_s(\rho).$$

This captures that the old contents of subsystem  $s$  are discarded (via partial trace), any prior entanglement across the cut  $(s, \bar{s})$  is destroyed, and a fresh local state  $\rho_s$  is prepared.

**Unitary application.** For `apply`  $U_s$  with  $U_s$  unitary on  $H_s$ ,

$$\llbracket \text{apply } U_s \rrbracket(\rho) := U_s^{(s)} \rho (U_s^{(s)})^\dagger.$$

This is conjugation by the cylindrically-extended unitary, i.e. “apply  $U_s$  locally on  $s$  and do nothing to  $\bar{s}$ .”

**Conditionals.** Let  $M_s = \{(m, M_m)\}_{m \in \text{Out}(M_s)}$  be a measurement on subsystem  $s$  in Kraus form (with  $\sum_m M_m^\dagger M_m = \mathbf{1}_{H_s}$ ). The command

$$\text{if } (\square m. M_s = m \rightarrow C_m) \text{ fi}$$

measures  $s$  and then executes  $C_m$  on the corresponding post-measurement state. Denotationally, because the measurement outcome is not returned as an explicit classical value, the overall output is the *sum* (mixture) of the branch outputs:

$$[\![\text{if } (\square m. M_s = m \rightarrow C_m) \text{ fi}]\!](\rho) := \sum_{m \in \text{Out}(M_s)} [\![C_m]\!]\left(M_m^{(s)} \rho (M_m^{(s)})^\dagger\right).$$

Each branch state  $M_m^{(s)} \rho (M_m^{(s)})^\dagger$  is subnormalized; its trace equals the probability mass of obtaining outcome  $m$  from the current partial state  $\rho$ . Summing over  $m$  therefore yields a single partial density operator that represents the full ensemble after the conditional.

## 6.1 While semantics: syntactic approximants and limits

A while-loop can, in general, iterate an unbounded number of times, so its semantics cannot be given by a finite structural recursion. CoqQ resolves this by defining the loop as the limit of an increasing sequence of *finite unrollings* (syntactic approximants). This construction is also standard in denotational accounts of classical while-languages.

**The loop and its measurement interface.** Fix a loop command

$$W \equiv \text{while } M'_s = 1 \text{ do } C \text{ od},$$

where  $M'_s = \{M_0, M_1\}$  is a two-outcome measurement on  $H_s$  (so  $M_0^\dagger M_0 + M_1^\dagger M_1 = \mathbf{1}_{H_s}$ ). Outcome 0 terminates the loop; outcome 1 executes the body  $C$  and repeats.

**Syntactic approximants.** Define commands  $W^{(n)}$  for integers  $n \geq 0$  by:

$$W^{(0)} := \text{abort},$$

and

$$W^{(n+1)} := \text{if } (\square b. M'_s = b \rightarrow D_b) \text{ fi}, \quad \text{where } D_0 := \text{skip}, \quad D_1 := C; W^{(n)}.$$

Intuitively,  $W^{(n)}$  represents “run the loop for at most  $n$  continue-iterations”: if we observe  $n$  consecutive outcomes 1, the approximant forces nontermination by falling back to `abort`. Thus,  $W^{(n)}$  captures exactly the contribution of executions that terminate within  $n$  loop-iterations.

Recall the Löwner order  $\sqsubseteq$  on Hermitian operators:  $A \sqsubseteq B$  iff  $B - A \succeq 0$ . It extends pointwise to super-operators by

$$\mathcal{E} \sqsubseteq \mathcal{F} \iff \forall \rho \succeq 0, \mathcal{E}(\rho) \sqsubseteq \mathcal{F}(\rho).$$

The approximants form an increasing chain in this order. Concretely, one can prove for every  $n \geq 0$  and every  $\rho \in \mathcal{D}_{\leq 1}(H)$  that  $[\![W^{(n)}]\!](\rho) \sqsubseteq [\![W^{(n+1)}]\!](\rho)$ .

The intuitive reason is simple: allowing one more unrolling can only add more terminating behaviors, hence more positive output mass. Moreover, each  $[\![W^{(n)}]\!](\rho)$  is bounded above by  $\rho$  in trace (indeed  $\text{tr}([\![W^{(n)}]\!](\rho)) \leq \text{tr}(\rho)$ ), so the chain is increasing but bounded.

**Defining the loop as a limit.** Because  $\{\llbracket W^{(n)} \rrbracket(\rho)\}_{n \geq 0}$  is a non-decreasing sequence of positive operators bounded in trace, it has a least upper bound in the Löwner order. CoqQ uses monotone convergence principles on ordered Hilbert spaces to justify that the pointwise limit exists and is again a well-defined super-operator. We therefore *define*:

$$\llbracket W \rrbracket(\rho) := \lim_{n \rightarrow \infty} \llbracket W^{(n)} \rrbracket(\rho).$$

Operationally,  $\llbracket W \rrbracket(\rho)$  is the total (subnormalized) output state contributed by all terminating executions of the loop, with the traces accounting for the total termination probability.

Since each approximant captures termination within  $n$  iterations, the scalar  $\text{tr}(\llbracket W^{(n)} \rrbracket(\rho))$  is the probability mass of terminating within  $n$  iterations from initial state  $\rho$ . Consequently, the limit

$$\text{tr}(\llbracket W \rrbracket(\rho)) = \lim_{n \rightarrow \infty} \text{tr}(\llbracket W^{(n)} \rrbracket(\rho))$$

is the total probability of termination of the loop on input  $\rho$ .

**Relation to domain-theoretic least fixed points.** A classical domain-theoretic semantics interprets a while-loop as a least fixed point of a functional on a CPO of state transformers. In the present setting, define the measurement super-operators

$$\mathcal{M}_b(\rho) := M_b^{(s)} \rho (M_b^{(s)})^\dagger \quad (b \in \{0, 1\}).$$

Then the loop equation informally reads:

$$\llbracket W \rrbracket(\rho) = \mathcal{M}_0(\rho) + \llbracket W \rrbracket(\llbracket C \rrbracket(\mathcal{M}_1(\rho))),$$

i.e. “stop on outcome 0, otherwise run  $C$  and loop again”. We will show that the limit-of-approximants definition above coincides with the standard least-fixed-point semantics, using a lemma that connects suprema of increasing chains of quantum operations with pointwise limits of super-operators.

**Why super-operators?** There are two complementary reasons to take *super-operators* as the semantic objects of qwhile commands.

First, super-operators are the mathematically natural level at which quantum programs compose. Every primitive command we allow—local unitary evolution, initialization (reset), and measurement followed by classical control—acts on density operators by an operation of the form

$$\rho \mapsto \sum_i E_i \rho E_i^\dagger,$$

possibly with a single Kraus operator (unitaries) or with a sum over branches (measurements and conditionals). This transformation is *linear* in  $\rho$  and is completely determined by the operators describing the physical action on the subsystem. Linearity is essential: it encodes the principle that a mixed input state (a probabilistic mixture of preparations) is transformed by the program into the corresponding mixture of outputs. As a result, sequential composition and program equivalence reduce to ordinary algebra of linear maps:

$$\llbracket C_1; C_2 \rrbracket = \llbracket C_2 \rrbracket \circ \llbracket C_1 \rrbracket.$$

Second, super-operators provide the right domain for giving a robust semantics of `while`. To interpret loops we need an order structure and a notion of limits for increasing chains of approximants. The Löwner order on positive operators lifts pointwise to super-operators, turning program denotations into an ordered space where one can define

$$\llbracket \text{while } M'_s = 1 \text{ do } C \text{ od} \rrbracket = \lim_{n \rightarrow \infty} \llbracket W^{(n)} \rrbracket,$$

and justify that this limit exists and yields a well-defined linear transformer. This ‘‘limit-of-approximants’’ viewpoint also aligns with the standard least-fixed-point semantics of while-programs, but avoids additional domain-theoretic machinery in the first presentation.

Finally, although the intended semantic objects are *quantum operations* (completely positive, trace-nonincreasing maps on density operators), it is technically convenient to define denotations at the broader super-operator level: it allows uniform linear-algebraic reasoning and smooth compositional definitions. One then proves, as a separate theorem, that every  $\llbracket C \rrbracket$  generated by the qwhile syntax is indeed a quantum operation.

**Theorem 6.1.** *For every command  $C$ , the denotation  $\llbracket C \rrbracket$  is a quantum operation (i.e., completely positive and trace-nonincreasing), and the loop semantics defined by the limit of syntactic approximants coincides with the standard domain-theoretic semantics (least fixed point in the CPO of quantum operations).*

**Lemma 6.2.** *If  $E, F \in \text{QO}(H)$ , then  $E \circ F \in \text{QO}(H)$ .*

*Proof.* CP:  $(E \circ F) \otimes I = (E \otimes I) \circ (F \otimes I)$ , and composition of positive maps is positive.  
TNI: for  $A \succeq 0$ ,

$$\text{tr}((E \circ F)(A)) = \text{tr}(E(F(A))) \leq \text{tr}(F(A)) \leq \text{tr}(A).$$

□

**Lemma 6.3.** *Kraus form implies quantum operation. That is, if*

$$E(A) = \sum_i K_i A K_i^\dagger \quad \text{and} \quad \sum_i K_i^\dagger K_i \preceq I,$$

*then  $E$  is CP and TNI (hence  $E \in \text{QO}(H)$ ).*

*Proof.* CP: immediate, since  $E \otimes I$  has Kraus operators  $\{K_i \otimes I\}$ .

TNI: for  $A \succeq 0$ ,

$$\text{tr}(E(A)) = \sum_i \text{tr}(K_i A K_i^\dagger) = \sum_i \text{tr}(K_i^\dagger K_i A) = \text{tr}\left(\left(\sum_i K_i^\dagger K_i\right) A\right) \leq \text{tr}(A).$$

□

**Definition 6.4.** For super-operators  $E, F : \mathcal{L}(H) \rightarrow \mathcal{L}(H)$ , define

$$E \sqsubseteq F \iff \forall A \succeq 0, E(A) \sqsubseteq F(A).$$

**Theorem 6.5.** *For every qwhile command  $C$ ,  $\llbracket C \rrbracket \in \text{QO}(H)$ .*

*Proof.* Recall that  $\text{QO}(H)$  denotes the set of *quantum operations* on  $H$ , i.e. super-operators  $\mathcal{E} : \mathcal{L}(H) \rightarrow \mathcal{L}(H)$  that are completely positive (CP) and trace-nonincreasing (TNI). We prove the claim by structural induction on the syntax of  $C$ .

*Case 1:*  $C = \text{error}$ . By definition,  $\llbracket \text{error} \rrbracket(\rho) = 0$  for all  $\rho$ . The zero map is CP (it preserves positivity even after tensoring with identities) and TNI since  $\text{tr}(0) = 0 \leq \text{tr}(\rho)$ . Hence  $\llbracket \text{error} \rrbracket \in \text{QO}(H)$ .

*Case 2:*  $C = \text{skip}$ .  $\llbracket \text{skip} \rrbracket(\rho) = \rho$ . The identity super-operator is CP and trace-preserving (hence TNI). So  $\llbracket \text{skip} \rrbracket \in \text{QO}(H)$ .

*Case 3:*  $C = C_1; C_2$ . By the denotational clause for sequencing,  $\llbracket C_1; C_2 \rrbracket = \llbracket C_2 \rrbracket \circ \llbracket C_1 \rrbracket$ , and by the lemma 6.2, we have  $\llbracket C_1; C_2 \rrbracket \in \text{QO}(H)$ .

*Case 4:*  $C = \text{init } \rho_s$ . Let  $s \subseteq \text{Reg}$  and write  $R := \bar{s}$ , so  $H \cong H_s \otimes H_R$ . By definition,

$$\llbracket \text{init } \rho_s \rrbracket(\rho) = \rho_s \otimes \text{tr}_s(\rho).$$

We show this map is a quantum operation by exhibiting Kraus operators.

Fix an orthonormal basis  $\{|i\rangle\}_i$  of  $H_s$  and a spectral decomposition

$$\rho_s = \sum_j p_j |\psi_j\rangle\langle\psi_j|, \quad p_j \geq 0, \quad \sum_j p_j = 1.$$

Define operators  $K_{ij} \in L(H_s \otimes H_R)$  by

$$K_{ij} := \sqrt{p_j} (|\psi_j\rangle\langle i| \otimes \mathbf{1}_{H_R}).$$

Then

$$K_{ij}^\dagger K_{ij} = p_j (|i\rangle\langle i| \otimes \mathbf{1}_{H_R}),$$

so

$$\sum_{i,j} K_{ij}^\dagger K_{ij} = \left( \sum_j p_j \right) \left( \sum_i |i\rangle\langle i| \right) \otimes \mathbf{1}_{H_R} = \mathbf{1}_{H_s} \otimes \mathbf{1}_{H_R} = \mathbf{1}.$$

Hence the induced map is CP and trace-preserving (thus TNI). Moreover, for any  $\rho$ ,

$$\begin{aligned} \sum_{i,j} K_{ij} \rho K_{ij}^\dagger &= \sum_{i,j} p_j (|\psi_j\rangle\langle i| \otimes \mathbf{1}) \rho (|i\rangle\langle\psi_j| \otimes \mathbf{1}) \\ &= \sum_j p_j \left( |\psi_j\rangle\langle\psi_j| \otimes \sum_i (|i\rangle\langle i| \otimes \mathbf{1}) \rho (|i\rangle\langle i| \otimes \mathbf{1}) \right) \\ &= \left( \sum_j p_j |\psi_j\rangle\langle\psi_j| \right) \otimes \text{tr}_s(\rho) \\ &= \rho_s \otimes \text{tr}_s(\rho). \end{aligned}$$

Thus  $\llbracket \text{init } \rho_s \rrbracket \in \text{QO}(H)$ .

*Case 5:  $C = \text{apply } U_s$ .* Let  $U_s$  be unitary on  $H_s$ . By definition,

$$\llbracket \text{apply } U_s \rrbracket(\rho) = U_s^{(s)} \rho (U_s^{(s)})^\dagger,$$

where  $U_s^{(s)} := U_s \otimes \mathbf{1}_{H_{\bar{s}}}$  is the cylindrical extension. This is a Kraus map with a single Kraus operator  $U_s^{(s)}$ , and  $(U_s^{(s)})^\dagger U_s^{(s)} = \mathbf{1}$ , so it is CP and trace-preserving (hence TNI). Therefore  $\llbracket \text{apply } U_s \rrbracket \in \text{QO}(H)$ .

*Case 6:  $C = \text{if } (\square m. M_s = m \rightarrow C_m) \text{ fi}$ .* Let  $M_s = \{(m, M_m)\}_{m \in \text{Out}(M_s)}$  be a measurement on  $H_s$  with  $\sum_m M_m^\dagger M_m = \mathbf{1}_{H_s}$ . By definition,

$$\llbracket \text{if } (\square m. M_s = m \rightarrow C_m) \text{ fi} \rrbracket(\rho) = \sum_{m \in \text{Out}(M_s)} \llbracket C_m \rrbracket \left( M_m^{(s)} \rho (M_m^{(s)})^\dagger \right).$$

*CP.* For each  $m$ , the map  $\rho \mapsto M_m^{(s)} \rho (M_m^{(s)})^\dagger$  is CP (single Kraus operator). By IH,  $\llbracket C_m \rrbracket$  is CP, and composition preserves CP. Finally, a finite sum of CP maps is CP. Hence the whole denotation is CP.

*TNI.* Let  $\rho \succeq 0$ . Using IH (each  $\llbracket C_m \rrbracket$  is TNI),

$$\text{tr} \left( \llbracket C_m \rrbracket \left( M_m^{(s)} \rho (M_m^{(s)})^\dagger \right) \right) \leq \text{tr} \left( M_m^{(s)} \rho (M_m^{(s)})^\dagger \right).$$

Summing over  $m$  gives

$$\begin{aligned} \text{tr} \left( \llbracket \text{if } \dots \text{ fi} \rrbracket(\rho) \right) &\leq \sum_m \text{tr} \left( M_m^{(s)} \rho (M_m^{(s)})^\dagger \right) \\ &= \text{tr} \left( \left( \sum_m (M_m^{(s)})^\dagger M_m^{(s)} \right) \rho \right) \\ &= \text{tr}(\rho), \end{aligned}$$

since  $\sum_m (M_m^{(s)})^\dagger M_m^{(s)} = \mathbf{1}$  (cylindrical extension preserves completeness). Therefore the denotation is TNI, hence in  $\text{QO}(H)$ .

*Case 7:  $C = \text{while } M'_s = 1 \text{ do } C_{\text{body}} \text{ od}$ .* Let  $M'_s = \{M_0, M_1\}$  be a two-outcome measurement on  $H_s$ . As in Section 6.1, define syntactic approximants  $W^{(n)}$  by

$$W^{(0)} := \text{abort}, \quad W^{(n+1)} := \text{if } (\square b. M'_s = b \rightarrow D_b) \text{ fi}, \quad D_0 := \text{skip}, \quad D_1 := C_{\text{body}}; W^{(n)}.$$

The loop denotation is defined by the increasing limit

$$\llbracket \text{while } M'_s = 1 \text{ do } C_{\text{body}} \text{ od} \rrbracket := \bigsqcup_{n \geq 0} \llbracket W^{(n)} \rrbracket = \lim_{n \rightarrow \infty} \llbracket W^{(n)} \rrbracket.$$

-each approximant denotes a quantum operation. We show  $\llbracket W^{(n)} \rrbracket \in \text{QO}(H)$  by induction on  $n$ . For  $n = 0$ ,  $W^{(0)} = \text{abort}$  and Case 1 applies. For the step  $n \mapsto n + 1$ , the command  $W^{(n+1)}$  is an if whose branches use only `skip` and  $C_{\text{body}}; W^{(n)}$ . By IH and Cases 2–6, the denotations of these constructs are in  $\text{QO}(H)$ , hence  $\llbracket W^{(n+1)} \rrbracket \in \text{QO}(H)$ .

-the approximant chain is nondecreasing. Write  $E_n := \llbracket W^{(n)} \rrbracket$ . Intuitively,  $W^{(n)}$  accounts for executions that terminate within at most  $n$  loop-iterations, so allowing  $n+1$  iterations can only add additional terminating probability mass. Formally, one shows (by induction on  $n$ ) that  $E_n \sqsubseteq E_{n+1}$  in the pointwise Löwner order on super-operators:

$$E_n \sqsubseteq E_{n+1} \iff \forall \rho \succeq 0, E_n(\rho) \sqsubseteq E_{n+1}(\rho).$$

**Lemma 6.6** (Approximants are nondecreasing). *Let  $W \equiv \text{while } M'_s = 1 \text{ do } C_{\text{body}} \text{ od}$  with  $M'_s = \{M_0, M_1\}$  a two-outcome measurement on  $H_s$ , and let  $W^{(n)}$  be the syntactic approximants as above. Write  $E_n := \llbracket W^{(n)} \rrbracket$ . Then  $E_n \sqsubseteq E_{n+1}$  for all  $n \geq 0$ , i.e.*

$$\forall n \geq 0, \quad \forall \rho \succeq 0, \quad E_n(\rho) \sqsubseteq E_{n+1}(\rho).$$

*Proof.* Fix  $n \geq 0$ . We first rewrite  $E_{n+1}$  in a convenient unfolded form.

*Unfolding.* By the denotational clause for if (specialized to outcomes  $b \in \{0, 1\}$ ) and using  $\llbracket \text{skip} \rrbracket(\rho) = \rho$  and  $\llbracket C_1; C_2 \rrbracket = \llbracket C_2 \rrbracket \circ \llbracket C_1 \rrbracket$ , we have for all  $\rho$ :

$$\begin{aligned} E_{n+1}(\rho) &= \llbracket D_0 \rrbracket \left( M_0^{(s)} \rho (M_0^{(s)})^\dagger \right) + \llbracket D_1 \rrbracket \left( M_1^{(s)} \rho (M_1^{(s)})^\dagger \right) \\ &= M_0^{(s)} \rho (M_0^{(s)})^\dagger + (E_n \circ \llbracket C_{\text{body}} \rrbracket) \left( M_1^{(s)} \rho (M_1^{(s)})^\dagger \right). \end{aligned} \tag{1}$$

Define two auxiliary (positive) maps on inputs  $\rho \succeq 0$ :

$$T(\rho) := M_0^{(s)} \rho (M_0^{(s)})^\dagger, \quad B(\rho) := \llbracket C_{\text{body}} \rrbracket \left( M_1^{(s)} \rho (M_1^{(s)})^\dagger \right).$$

Then (1) becomes simply

$$E_{n+1}(\rho) = T(\rho) + E_n(B(\rho)). \tag{2}$$

Similarly,

$$E_{n+2}(\rho) = T(\rho) + E_{n+1}(B(\rho)). \tag{3}$$

*Positivity facts.* If  $\rho \succeq 0$ , then  $T(\rho) \succeq 0$  because  $\rho \mapsto M_0^{(s)} \rho (M_0^{(s)})^\dagger$  is a (single-Kraus) CP map. Also  $B(\rho) \succeq 0$  because  $\rho \mapsto M_1^{(s)} \rho (M_1^{(s)})^\dagger$  is CP and  $\llbracket C_{\text{body}} \rrbracket$  is CP by the outer induction hypothesis on program structure (the body is a strict subcommand of the loop).

*Induction on  $n$ .* We prove  $E_n \sqsubseteq E_{n+1}$  for all  $n$  by induction on  $n$ .

Base  $n = 0$ .  $E_0 = \llbracket W^{(0)} \rrbracket = \llbracket \text{error} \rrbracket$ , hence  $E_0(\rho) = 0$  for all  $\rho$ . Since  $E_1(\rho) \succeq 0$  for all  $\rho \succeq 0$  (by (2) with  $n = 0$ ), we have  $E_0(\rho) = 0 \sqsubseteq E_1(\rho)$ .

Step. Assume  $E_n \sqsubseteq E_{n+1}$ , i.e. for all  $X \succeq 0$ ,  $E_n(X) \sqsubseteq E_{n+1}(X)$ . We must show  $E_{n+1} \sqsubseteq E_{n+2}$ . Fix any  $\rho \succeq 0$ . Then  $B(\rho) \succeq 0$ , so applying the induction hypothesis to  $X = B(\rho)$  yields

$$E_n(B(\rho)) \sqsubseteq E_{n+1}(B(\rho)).$$

Adding the same positive operator  $T(\rho)$  to both sides preserves the Löwner order, hence

$$T(\rho) + E_n(B(\rho)) \sqsubseteq T(\rho) + E_{n+1}(B(\rho)).$$

Using (2) and (3), this is exactly  $E_{n+1}(\rho) \sqsubseteq E_{n+2}(\rho)$ .

Thus  $E_n \sqsubseteq E_{n+1}$  for all  $n \geq 0$ .  $\square$

-increasing limits preserve being a quantum operation. Since each  $E_n$  is CP and TNI and  $(E_n)$  is nondecreasing, the pointwise supremum  $E := \bigsqcup_{n \geq 0} E_n$  exists (in finite dimension) and remains CP and TNI. Equivalently,  $E$  is a quantum operation and is the least upper bound of the chain.

**Lemma 6.7.** *Let  $(E_n)_{n \geq 0}$  be a nondecreasing chain in  $\text{QO}(H)$ , i.e.*

$$\forall n, \quad E_n \sqsubseteq E_{n+1} \iff \forall \rho \succeq 0, \quad E_n(\rho) \sqsubseteq E_{n+1}(\rho).$$

*Then the pointwise supremum*

$$E := \bigsqcup_{n \geq 0} E_n$$

*exists, is the least upper bound of the chain, and satisfies  $E \in \text{QO}(H)$  (hence  $E$  is CP and TNI).*

*Proof.* Because  $H$  is finite-dimensional, we can use the Choi–Jamiołkowski representation.

-Choi matrices and their order. Fix an orthonormal basis  $\{|i\rangle\}_{i=1}^d$  of  $H$  and let

$$|\Omega\rangle := \sum_{i=1}^d |i\rangle \otimes |i\rangle \in H \otimes H.$$

For a super-operator  $\mathcal{E} : L(H) \rightarrow L(H)$  define its Choi matrix

$$J(\mathcal{E}) := (\mathcal{E} \otimes \mathbf{1})(|\Omega\rangle\langle\Omega|) \in L(H \otimes H).$$

We use the following standard facts (Choi's theorem and its trace characterization):

$\mathcal{E}$  is CP iff  $J(\mathcal{E}) \succeq 0$ .

$\mathcal{E}$  is TNI iff  $\text{tr}_1(J(\mathcal{E})) \preceq \mathbf{1}$ , where  $\text{tr}_1$  denotes the partial trace over the *first* tensor factor of  $H \otimes H$ .

The assignment  $\mathcal{E} \mapsto J(\mathcal{E})$  is linear and injective, hence determines  $\mathcal{E}$  uniquely from  $J(\mathcal{E})$ .

Write  $J_n := J(E_n)$ . Since each  $E_n$  is CP, we have  $J_n \succeq 0$  for all  $n$ . Moreover,  $E_n \sqsubseteq E_{n+1}$  implies  $J_n \sqsubseteq J_{n+1}$  because

$$J_{n+1} - J_n = ((E_{n+1} - E_n) \otimes \mathbf{1})(|\Omega\rangle\langle\Omega|) \succeq 0$$

(the map  $E_{n+1} - E_n$  is positive by definition of  $\sqsubseteq$ , hence so is its tensor extension). Thus  $(J_n)$  is an increasing sequence in the Löwner order.

-boundedness and existence of the limit. Each  $E_n$  is TNI, so  $\text{tr}_1(J_n) \preceq \mathbf{1}$ . Taking trace and using  $\text{tr}(J_n) = \text{tr}(\text{tr}_1(J_n))$ , we obtain a uniform trace bound:

$$\text{tr}(J_n) = \text{tr}(\text{tr}_1(J_n)) \leq \text{tr}(\mathbf{1}) = d \quad \text{for all } n.$$

Hence  $(J_n)$  is an increasing sequence of PSD operators with uniformly bounded trace. In finite dimension this implies convergence: there exists a PSD operator  $J$  such that

$$J = \lim_{n \rightarrow \infty} J_n \quad \text{and} \quad J_n \sqsubseteq J \quad \text{for all } n.$$

(One way to see this is that the eigenvalues of  $J_n$  increase monotonically but their sum is bounded by  $d$ , so each eigenvalue converges; equivalently, the cone of PSD matrices is closed and increasing bounded sequences converge.)

-define  $E$  by the limit Choi matrix. By injectivity of the Choi representation, there is a unique linear map  $E : L(H) \rightarrow L(H)$  such that

$$J(E) = J.$$

We claim  $E$  is exactly the least upper bound  $\bigsqcup_n E_n$ .

- $E$  is CP and TNI. Since  $J \succeq 0$ , Choi's theorem gives that  $E$  is CP. Also, partial trace is continuous, so

$$\mathrm{tr}_1(J) = \mathrm{tr}_1\left(\lim_{n \rightarrow \infty} J_n\right) = \lim_{n \rightarrow \infty} \mathrm{tr}_1(J_n) \preceq \mathbf{1},$$

because each  $\mathrm{tr}_1(J_n) \preceq \mathbf{1}$ . Thus  $E$  is TNI. Therefore  $E \in \mathrm{QO}(H)$ .

*Step 5:  $E$  is the least upper bound of  $(E_n)$ .* First,  $E$  is an upper bound. Indeed,  $J_n \sqsubseteq J$  implies  $J(E - E_n) = J - J_n \succeq 0$ , hence  $E - E_n$  is CP and therefore positive. Thus for all  $\rho \succeq 0$ ,

$$E_n(\rho) \sqsubseteq E(\rho),$$

i.e.  $E_n \sqsubseteq E$ .

Second,  $E$  is the least upper bound. Let  $F$  be any upper bound, so  $E_n \sqsubseteq F$  for all  $n$ . Then  $J_n = J(E_n) \sqsubseteq J(F)$  for all  $n$ , hence taking  $n \rightarrow \infty$  yields  $J = \lim_n J_n \sqsubseteq J(F)$ . Therefore  $J(F - E) = J(F) - J(E) \succeq 0$ , so  $F - E$  is CP and  $E \sqsubseteq F$ . This shows  $E$  is the least upper bound.

Hence the pointwise supremum  $E = \bigsqcup_{n \geq 0} E_n$  exists and belongs to  $\mathrm{QO}(H)$ .  $\square$

Therefore the loop denotation (defined as this supremum) lies in  $\mathrm{QO}(H)$ .  $\square$

## 6.2 The domain-theoretic setup

The paper contrasts its loop semantics (a limit of syntactic approximants) with the classic domain-theoretic semantics (a least fixed point in a CPO of quantum operations), and then claims that the two coincide. We now prove this coincidence in our setting.

The “classic” approach assumes  $(\mathrm{QO}(H), \sqsubseteq)$  is a CPO and that the loop functional is Scott-continuous, so that least fixed points exist and can be obtained via the Kleene construction.

In our concrete finite-dimensional setting, we do not need to assume these abstract facts. We already proved the key concrete statement we need: for any nondecreasing  $\omega$ -chain of quantum operations, the pointwise supremum exists and yields a quantum operation (Lemma 6.7), and this supremum agrees with the corresponding operator limit.

**Bottom element.** Let  $\perp$  be the zero super-operator:

$$\perp(\rho) := 0.$$

Then  $\perp \sqsubseteq E$  for every positive map  $E$ , hence  $\perp$  is the least element of  $(\mathrm{QO}(H), \sqsubseteq)$ .

**The loop functional.** Fix a loop command in qwhile notation:

$$W \equiv \text{while } M'_s = 1 \text{ do } C_{\text{body}} \text{ od},$$

where  $M'_s = \{M_0, M_1\}$  is a two-outcome measurement on subsystem  $s$ . (Outcome 0 terminates; outcome 1 continues.)

Define a functional  $\Phi : \text{QO}(H) \rightarrow \text{QO}(H)$  by

$$\Phi(X)(\rho) := M_0^{(s)} \rho (M_0^{(s)})^\dagger + X(\llbracket C_{\text{body}} \rrbracket (M_1^{(s)} \rho (M_1^{(s)})^\dagger)).$$

This is the denotation of the one-step unfolding of the loop: measure the guard; if outcome is 0, stop; if outcome is 1, execute the body and then “recur”, with the recursive call represented by the parameter  $X$ .

**Lemma 6.8.**  $\Phi$  maps  $\text{QO}(H)$  to  $\text{QO}(H)$ .

*Proof.* Fix  $X \in \text{QO}(H)$ . We show  $\Phi(X) \in \text{QO}(H)$ .

*CP.* The map  $\rho \mapsto M_0^{(s)} \rho (M_0^{(s)})^\dagger$  is CP (single Kraus operator). The map  $\rho \mapsto \llbracket C_{\text{body}} \rrbracket (M_1^{(s)} \rho (M_1^{(s)})^\dagger)$  is a composition of quantum operations (apply a Kraus map, then  $\llbracket C_{\text{body}} \rrbracket$ ), hence is CP. Composing with  $X$  preserves CP, and a finite sum of CP maps is CP. Thus  $\Phi(X)$  is CP.

*TNI.* Let  $\rho \succeq 0$ . Using that  $X$  is TNI and  $\llbracket C_{\text{body}} \rrbracket$  is TNI (Theorem 6.5), we obtain

$$\begin{aligned} \text{tr}(\Phi(X)(\rho)) &= \text{tr}\left(M_0^{(s)} \rho (M_0^{(s)})^\dagger\right) + \text{tr}\left(X(\llbracket C_{\text{body}} \rrbracket (M_1^{(s)} \rho (M_1^{(s)})^\dagger))\right) \\ &\leq \text{tr}\left(M_0^{(s)} \rho (M_0^{(s)})^\dagger\right) + \text{tr}\left(\llbracket C_{\text{body}} \rrbracket (M_1^{(s)} \rho (M_1^{(s)})^\dagger)\right) \\ &\leq \text{tr}\left(M_0^{(s)} \rho (M_0^{(s)})^\dagger\right) + \text{tr}\left(M_1^{(s)} \rho (M_1^{(s)})^\dagger\right) \\ &= \text{tr}\left((M_0^{(s)})^\dagger M_0^{(s)} + (M_1^{(s)})^\dagger M_1^{(s)})\rho\right) \\ &= \text{tr}(\rho), \end{aligned}$$

since  $(M_0^{(s)})^\dagger M_0^{(s)} + (M_1^{(s)})^\dagger M_1^{(s)} = \mathbf{1}$  by measurement completeness (cylindrical extension preserves the identity). So  $\Phi(X)$  is TNI. Hence  $\Phi(X) \in \text{QO}(H)$ .  $\square$

**Approximants are iterates of  $\Phi$  from  $\perp$ .** Let  $(W^{(n)})_{n \geq 0}$  be the syntactic approximants for the loop  $W$  defined earlier:

$$W^{(0)} := \text{error}, \quad W^{(n+1)} := \text{if } (\square b. M'_s = b \rightarrow D_b) \text{ fi}, \quad D_0 := \text{skip}, \quad D_1 := C_{\text{body}}; W^{(n)}.$$

Write  $E_n := \llbracket W^{(n)} \rrbracket \in \text{QO}(H)$ .

**Lemma 6.9.**  $E_0 = \perp$  and  $E_{n+1} = \Phi(E_n)$  for all  $n \geq 0$ .

*Proof.* By denotation of `error`,  $E_0 = \llbracket \text{error} \rrbracket = \perp$ .

For the step, expand  $E_{n+1}$  using the denotational clauses for `if`, `skip`, and sequencing:

$$\begin{aligned} E_{n+1}(\rho) &= \llbracket \text{skip} \rrbracket \left( M_0^{(s)} \rho (M_0^{(s)})^\dagger \right) + \llbracket C_{\text{body}}; W^{(n)} \rrbracket \left( M_1^{(s)} \rho (M_1^{(s)})^\dagger \right) \\ &= M_0^{(s)} \rho (M_0^{(s)})^\dagger + E_n \left( \llbracket C_{\text{body}} \rrbracket (M_1^{(s)} \rho (M_1^{(s)})^\dagger) \right) \\ &= \Phi(E_n)(\rho). \end{aligned}$$

Thus  $E_{n+1} = \Phi(E_n)$ . In particular, for all  $n$ ,  $E_n = \Phi^n(\perp)$ .  $\square$

The classic domain-theoretic semantics of the loop is the least fixed point

$$\text{lfp}(\Phi),$$

taken in  $(\text{QO}(H), \sqsubseteq)$ . The Kleene construction says that, for a Scott-continuous (or at least  $\omega$ -continuous)  $\Phi$ ,

$$\text{lfp}(\Phi) = \bigsqcup_{n \geq 0} \Phi^n(\perp).$$

We now show directly that the supremum of the approximant denotations is a least fixed point of  $\Phi$ .

**Lemma 6.10.** *Let  $E_n := \llbracket W^{(n)} \rrbracket$  and define*

$$E := \bigsqcup_{n \geq 0} E_n.$$

*Then  $E$  is a fixed point of  $\Phi$  and is the least fixed point of  $\Phi$  in  $(\text{QO}(H), \sqsubseteq)$ .*

*Proof.* By Lemma 6.6,  $E_n \sqsubseteq E_{n+1}$  for all  $n$ . By Lemma 6.7, the supremum  $E = \bigsqcup_{n \geq 0} E_n$  exists and belongs to  $\text{QO}(H)$ .

*$E$  is a fixed point of  $\Phi$ .* Using Lemma 6.9,  $E_{n+1} = \Phi(E_n)$  for all  $n$ . Taking suprema of both sides yields

$$\bigsqcup_{n \geq 0} E_{n+1} = \bigsqcup_{n \geq 0} \Phi(E_n).$$

Since shifting an  $\omega$ -chain does not change its supremum,  $\bigsqcup_{n \geq 0} E_{n+1} = \bigsqcup_{n \geq 0} E_n = E$ . So it remains to show

$$\Phi\left(\bigsqcup_{n \geq 0} E_n\right) = \bigsqcup_{n \geq 0} \Phi(E_n).$$

Fix  $\rho \succeq 0$ . Write

$$T(\rho) := M_0^{(s)} \rho (M_0^{(s)})^\dagger, \quad B(\rho) := \llbracket C_{\text{body}} \rrbracket (M_1^{(s)} \rho (M_1^{(s)})^\dagger).$$

Then

$$\Phi(X)(\rho) = T(\rho) + X(B(\rho)).$$

Using the pointwise definition of supremum in the Löwner order,

$$E(B(\rho)) = \bigsqcup_{n \geq 0} E_n(B(\rho)).$$

Adding the fixed positive operator  $T(\rho)$  preserves suprema:

$$T(\rho) + E(B(\rho)) = \bigsqcup_{n \geq 0} (T(\rho) + E_n(B(\rho))).$$

But  $T(\rho) + E_n(B(\rho)) = \Phi(E_n)(\rho)$ , hence

$$\Phi(E)(\rho) = \bigsqcup_{n \geq 0} \Phi(E_n)(\rho).$$

Since this holds for all  $\rho \succeq 0$ , we conclude  $\Phi(E) = \bigsqcup_{n \geq 0} \Phi(E_n)$ . Combining with  $\bigsqcup_{n \geq 0} \Phi(E_n) = \bigsqcup_{n \geq 0} E_{n+1} = E$ , we obtain  $\Phi(E) = E$ .

*Step 3:  $E$  is the least fixed point.* Let  $F \in \text{QO}(H)$  be any fixed point,  $\Phi(F) = F$ . Since  $\perp \sqsubseteq F$  and  $\Phi$  is monotone, we have by induction

$$E_n = \Phi^n(\perp) \sqsubseteq \Phi^n(F) = F \quad \text{for all } n.$$

Taking suprema over  $n$  yields  $E = \bigsqcup_{n \geq 0} E_n \sqsubseteq F$ . Therefore  $E$  is the least fixed point of  $\Phi$ .  $\square$