Quantum Programming Languages and Semantics

5 QWhile Language

This section introduces the core programming language we will use for quantum program logics. The language follows the *classical control + quantum data* paradigm: the program's control flow (sequencing, branching, looping, and the program counter itself) is entirely classical, while the data manipulated by commands are quantum states (density operators) on a fixed composite Hilbert space. Concretely:

> *Control is classical.* The program counter is never put into superposition. The only source of probabilistic branching is *measurement*: a measurement produces a classical outcome, and the next command is chosen based on that outcome.
>
> *Data is quantum.* At every point, the program carries a (possibly subnormalized) density operator ρ on a fixed global Hilbert space H. Primitive commands act *locally* on specified subsystems, leaving the rest untouched (up to the standard identity extension).

Registers and subsystem structure. Fix a finite set of register labels Reg and a family of finite-dimensional Hilbert spaces $\{H_x\}_{x\in\mathsf{Reg}}$. The *global* state space is the tensor product

$$H \;\cong\; \bigotimes_{x\in\mathsf{Reg}} H_x.$$

A *subsystem* is a subset of labels $s \subseteq \mathsf{Reg}$. We write

$$H_s \;\cong\; \bigotimes_{x\in s} H_x, \qquad \overline{s} := \mathsf{Reg}\setminus s, \qquad H \cong H_s \otimes H_{\overline{s}}.$$

The purpose is to make precise the standard programming intuition that a program acts on *named registers* and typically touches only *finitely many* of them. A concrete quantum program is written in terms of a finite collection of variables/registers/qubits, such as $q_1, q_2, \ldots, q_n$, and every primitive command (unitary gates, measurements, initialization) targets a specified subset of these registers. Thus it is natural to model the program's data state as a single density operator on a tensor product space that factors according to these register boundaries. Moreover, working with explicit subsystems is essential for two semantic reasons:

> *Locality of commands.* A command that is declared to act on subsystem s should leave the rest of the machine state unchanged; this is expressed later by cylindrical extension ($A^{(s)} = A \otimes \mathbf{1}_{H_{\overline{s}}}$).
>
> *Discarding and re-initialization.* Initialization/reset operations need to "forget" whatever was previously stored in a register (including any entanglement with other registers). This is naturally described using the decomposition $H \cong H_s \otimes H_{\overline{s}}$ together with partial trace.

We fix a tensor-factor ordering/parenthesization convention so that expressions such as $H \cong H_s \otimes H_{\overline{s}}$ are well-defined (up to canonical unitary isomorphism). This lets us speak cleanly about commands that act only on s while leaving $\overline{s}$ unchanged.

Program states (subnormalized density operators). To represent probabilistic branching without constantly renormalizing, we use *subnormalized* (partial) density operators:

$$\mathcal{D}^{-}(H) \;:=\; \{\rho \in L(H) \;:\; \rho \sqsupseteq 0 \;\wedge\; \mathrm{tr}(\rho) \le 1\}.$$

Intuitively, $\mathrm{tr}(\rho)$ is the *probability mass* of reaching ρ along a particular execution path. Thus the same symbolic ρ can simultaneously encode the post-state *and* the probability of being in that post-state. The zero operator 0 is allowed and represents an impossible (unreachable) state.

A key design principle is *locality*: commands target a subsystem $s \subseteq \mathsf{Reg}$ and act as the identity on the complement $\overline{s}$. If $A \in L(H_s)$ is a linear operator acting on subsystem s, its *cylindrical extension* (identity extension) to the global space is

$$A^{(s)} := A \otimes \mathbf{1}_{H_{\overline{s}}} \quad \text{(under the fixed identification } H \cong H_s \otimes H_{\overline{s}}\text{)}.$$

Likewise, if U_s is unitary on H_s, then $U_s^{(s)}$ is unitary on H and represents "apply U_s on subsystem s and do nothing elsewhere."

We also need a primitive way to *discard* part of a composite system. For $\rho \in L(H)$ and $s \subseteq \mathsf{Reg}$, write $\mathrm{tr}_s(\rho)$ for the partial trace over H_s. Then $\mathrm{tr}_s(\rho) \in L(H_{\overline{s}})$ and preserves subnormalization:

$$\mathrm{tr}(\mathrm{tr}_s(\rho)) = \mathrm{tr}(\rho).$$

Operationally, tr_s means "throw away subsystem s and keep only the reduced state of the rest." A key operation in qwhile is to *discard* the old content of subsystem s and replace it by a fresh local state ρ_s on H_s. Intuitively, we first "throw away" subsystem s by taking the partial trace $\mathrm{tr}_s(\rho)$, and then prepare a new state ρ_s on s. As a result, the register s is set to ρ_s regardless of its previous contents, and any entanglement between s and $\overline{s}$ is removed. This is the subsystem-level generalization of the familiar qubit reset command $q := |0\rangle$.

5.1 QWhile Language

We now define a core language, *qwhile*, that is expressive enough to support quantum Hoare-style correctness reasoning and under-approximate incorrectness reasoning. The distinctive features are: (i) commands act on designated subsystems; (ii) branching/looping is controlled by measurement outcomes; (iii) the statement error models an explicit abnormal termination.

Definition 5.1. Fix a global register set Reg and global space $H \cong \bigotimes_{x \in \mathsf{Reg}} H_x$. qwhile commands are generated by the following grammar:

$$\begin{aligned} C \in \mathsf{Cmd} \quad ::= \quad & \mathsf{error} \mid \mathsf{skip} \mid C_1; C_2 \mid \mathsf{init}\ \rho_s \mid \mathsf{apply}\ U_s \\ & \mid \mathsf{if}\ (\Box m.\ M_s = m \to C_m)\ \mathsf{fi} \mid \mathsf{while}\ M'_s = 1\ \mathsf{do}\ C\ \mathsf{od}. \end{aligned}$$

Here: $s \subseteq \mathsf{Reg}$ ranges over subsystems. ρ_s ranges over density operators on H_s (i.e. $\rho_s \succeq 0$, $\mathrm{tr}(\rho_s) = 1$). U_s ranges over unitary operators on H_s. $M_s = \{(m, M_m)\}_{m \in \mathsf{Out}(M_s)}$ is a measurement on H_s in Kraus form, i.e. $\sum_m M_m^\dagger M_m = \mathbf{1}_{H_s}$. $M'_s = \{M_0, M_1\}$ is a two-outcome measurement on H_s (a special case of the above).

skip terminates normally and leaves the state unchanged.

error terminates *abnormally.* It is intended to model bug signals such as failed runtime checks. Crucially, once error occurs, the program stops immediately: any remaining code is discarded rather than executed.

$C_1; C_2$ is sequential composition: execute C_1 first; if C_1 terminates normally then continue with C_2; if C_1 terminates abnormally then the whole composition terminates abnormally.

$\mathsf{init}\ \rho_s$ *resets* subsystem s to ρ_s, discarding any prior content of s (including entanglement with $\overline{s}$). Operationally, it applies $\rho \mapsto \rho_s \otimes \mathrm{tr}_s(\rho)$.

$\mathsf{apply}\ U_s$ applies the unitary U_s to subsystem s (lifted cylindrically to H), i.e. $\rho \mapsto U_s^{(s)}\, \rho\, \big(U_s^{(s)}\big)^\dagger$.

$\mathsf{if}(\square m.\ M_s = m \to C_m)\mathsf{fi}$ first measures subsystem s using the measurement M_s. The (classical) outcome m selects the branch C_m, and the quantum state is updated by the corresponding Kraus operator M_m.

$\mathsf{while}\ M'_s = 1\ \mathsf{do}\ C\ \mathsf{od}$ repeatedly measures subsystem s using $M'_s = \{M_0, M_1\}$. Outcome 0 terminates the loop; outcome 1 executes the body C and repeats.

5.2 Operational semantics

The semantics is given as a labelled transition system on configurations. Exit conditions are

$$\epsilon ::= \mathsf{ok} \mid \mathsf{er},$$

where ok denotes normal steps/termination and er denotes abnormal termination caused by error. We call outputs of ok-terminations *normal states* and outputs of er-terminations *abnormal states.*

A *configuration* is a pair $\langle C, \rho\rangle$ where C is the remaining code to be executed (or $\downarrow$ to denote termination by convention) and $\rho \in \mathcal{D}^-(H)$ is the current program state. The one-step transition relation is written

$$\langle C, \rho\rangle \xrightarrow{\epsilon} \langle C', \rho'\rangle.$$

Because measurements branch on outcomes, a configuration may have multiple ok-successors, each carrying a different (subnormalized) post-measurement state.

Conventions. Whenever an operator is defined only on a subsystem s, it is understood to act on the whole space via cylindrical extension (e.g. $U_s^{(s)}$ and $M_m^{(s)}$). All rules below are to be understood under the fixed identification $H \cong H_s \otimes H_{\overline{s}}$ whenever subsystem s is involved, and with cylindrical extensions $A^{(s)} := A \otimes \mathbf{1}_{H_{\overline{s}}}$.

$$\frac{}{\langle \mathsf{skip}, \rho\rangle \xrightarrow{\mathsf{ok}} \langle \downarrow, \rho\rangle}\ (\textsc{Skip}) \qquad \frac{}{\langle \mathsf{error}, \rho\rangle \xrightarrow{\mathsf{er}} \langle \downarrow, \rho\rangle}\ (\textsc{Error})$$

The Error rule is the essence of abnormal termination: it stops execution immediately, raises label er, and returns the current quantum state unchanged.

$$\frac{\langle C_1, \rho\rangle \xrightarrow{\mathsf{ok}} \langle \downarrow, \rho'\rangle}{\langle C_1; C_2, \rho\rangle \xrightarrow{\mathsf{ok}} \langle C_2, \rho'\rangle}\ (\textsc{Seq-Done}) \qquad \frac{\langle C_1, \rho\rangle \xrightarrow{\mathsf{ok}} \langle C_1', \rho'\rangle}{\langle C_1; C_2, \rho\rangle \xrightarrow{\mathsf{ok}} \langle C_1'; C_2, \rho'\rangle}\ (\textsc{Seq-Step})$$

$$\frac{\langle C_1, \rho\rangle \xrightarrow{\mathsf{er}} \langle \downarrow, \rho'\rangle}{\langle C_1; C_2, \rho\rangle \xrightarrow{\mathsf{er}} \langle \downarrow, \rho'\rangle}\ (\textsc{Seq-Err})$$

These sequencing rules express two behaviors: (i) normal sequencing proceeds by stepping C_1 until it finishes, then continues with C_2; (ii) er *short-circuits* sequencing: if C_1 terminates abnormally, then the whole program terminates abnormally and C_2 is discarded.

$$\frac{}{\langle \mathsf{init}\ \rho_s, \rho\rangle \xrightarrow{\mathsf{ok}} \langle \downarrow, \rho_s \otimes \mathrm{tr}_s(\rho)\rangle}\ (\textsc{Init}) \qquad \frac{}{\langle \mathsf{apply}\ U_s, \rho\rangle \xrightarrow{\mathsf{ok}} \langle \downarrow, U_s^{(s)}\, \rho\, \big(U_s^{(s)}\big)^\dagger\rangle}\ (\textsc{Apply})$$

The Init rule makes explicit that initialization *forgets* whatever was stored in s by taking $\mathrm{tr}_s(\rho)$ and then prepares ρ_s afresh. The Apply rule is local unitary evolution: it preserves trace, so $\mathrm{tr}(\rho)$ (the path weight) is unchanged.

$$\frac{}{\langle \mathsf{if}\ (\Box m.\ M_s = m \to C_m)\ \mathsf{fi},\ \rho\rangle \xrightarrow{\mathsf{ok}} \langle C_m,\ M_m^{(s)}\,\rho\,\big(M_m^{(s)}\big)^{\dagger}\rangle, \qquad m \in \mathsf{Out}(M_s)}\ (\textsc{If})$$

This rule formalizes *measurement-controlled branching.* For each possible outcome m, there is a transition to the corresponding branch C_m. The post-measurement state is subnormalized: its trace equals the probability mass of seeing outcome m on input ρ.

$$\frac{}{\langle \mathsf{while}\ M'_s = 1\ \mathsf{do}\ C\ \mathsf{od},\ \rho\rangle \xrightarrow{\mathsf{ok}} \langle \downarrow,\ M_0^{(s)}\,\rho\,\big(M_0^{(s)}\big)^{\dagger}\rangle}\ (\textsc{While-0})$$

$$\frac{}{\langle \mathsf{while}\ M'_s = 1\ \mathsf{do}\ C\ \mathsf{od},\ \rho\rangle \xrightarrow{\mathsf{ok}} \langle C;\ \mathsf{while}\ M'_s = 1\ \mathsf{do}\ C\ \mathsf{od},\ M_1^{(s)}\,\rho\,\big(M_1^{(s)}\big)^{\dagger}\rangle}\ (\textsc{While-1})$$

The loop is driven by a two-outcome measurement. Outcome 0 terminates the loop immediately; outcome 1 unrolls one iteration: execute C and then repeat the loop.

Comments on normalization and probability. The rules intentionally avoid renormalization. For example, $M_m^{(s)}\rho(M_m^{(s)})^{\dagger}$ is not divided by its trace. Instead, $\mathrm{tr}\Big(M_m^{(s)}\rho(M_m^{(s)})^{\dagger}\Big)$ *is* the probability mass of taking outcome m from state ρ. This is why subnormalized states are convenient: the branching structure is classical (one successor per outcome), while the quantitative weights are carried by the traces of the resulting partial states.

Write $\xrightarrow{\epsilon}^{*}$ for the reflexive-transitive closure of $\xrightarrow{\epsilon}$, where the label records whether an abnormal termination occurred:

$\langle C,\ \rho\rangle \xrightarrow{\mathsf{ok}}^{*} \langle C',\ \rho'\rangle$ means: execute zero or more steps, and no step is labelled er.

$\langle C,\ \rho\rangle \xrightarrow{\mathsf{er}}^{*} \langle \downarrow,\ \rho'\rangle$ means: along the execution, an er-labelled termination occurs. By Seq-Err, once er happens, the remaining code is discarded and the computation ends immediately.

This separation of ok vs. er executions is essential for later incorrectness-style specifications: it allows us to talk about *normal outcomes* and *error outcomes* of the same program, and to treat the existence of an er-path as evidence of a bug.