# Foundations of Quantum Programming 

## Lecture 3: Syntax and Semantics of Quantum Programs

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## Outline

Syntax

Operational Semantics

Denotational Semantics

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Syntax

Operational Semantics

Denotational Semantics


$$
\begin{aligned}
S::=\text { skip } & |u:=t| S_{1} ; S_{2} \\
& \mid \text { if } b \text { then } S_{1} \text { else } S_{2} \text { fi } \\
& \mid \text { while } b \text { do } S \text { od. }
\end{aligned}
$$

- The conditional statement can be generalised to the case statement:

$$
\begin{aligned}
& \text { if } G_{1} \rightarrow S_{1} \\
& \square G_{2} \rightarrow S_{2} \\
& \quad \ldots . . \\
& \square G_{n} \rightarrow S_{n} \\
& \text { fi }
\end{aligned}
$$

or more compactly

$$
\text { if }\left(\square i \cdot G_{i} \rightarrow S_{i}\right) \mathbf{f i}
$$

## Quantum while-Language

- Fix the alphabet of quantum while-language: A countably infinite set $q$ Var of quantum variables. Symbols $q, q^{\prime}, q_{0}, q_{1}, q_{2}, \ldots$ denote quantum variables.


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\text { Boolean }=\mathcal{H}_{2}, \quad \text { integer }=\mathcal{H}_{\infty}
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- A quantum register is a finite sequence $\bar{q}=q_{1}, \ldots, q_{n}$ of distinct quantum variables. Its state Hilbert space:

$$
\mathcal{H}_{\bar{q}}=\bigotimes_{i=1}^{n} \mathcal{H}_{q_{i}} .
$$

## Quantum Programs

$$
\begin{aligned}
S::=\text { skip } & |q:=| 0\rangle|\bar{q}:=U[\bar{q}]| S_{1} ; S_{2} \\
& \mid \text { if }\left(\square m \cdot M[\bar{q}]=m \rightarrow S_{m}\right) \text { fi } \\
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- The control flow in the loop is classical too.
- Programs with quantum control flow?


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## Denotational Semantics

## Notations

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- Let $\bar{q}=q_{1}, \ldots, q_{n}$ be a quantum register. An operator $A$ in the state Hilbert space $\mathcal{H}_{\bar{q}}$ of $\bar{q}$ has a cylindrical extension $A \otimes I$ in $\mathcal{H}_{\text {all }}$.


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- A transition between quantum configurations:

$$
\langle S, \rho\rangle \rightarrow\left\langle S^{\prime}, \rho^{\prime}\right\rangle
$$

## Operational Semantics

The operational semantics of quantum programs is the transition relation $\rightarrow$ between quantum configurations defined by the transition rules:
(SK)

$$
\overline{\langle\mathbf{k k i p}, \rho\rangle \rightarrow\langle E, \rho\rangle}
$$

(IN)

$$
\overline{\langle q:=\mid 0\rangle, \rho\rangle \rightarrow\left\langle E, \rho_{0}^{q}\right\rangle}
$$

where

$$
\rho_{0}^{q}= \begin{cases}|0\rangle_{q}\langle 0| \rho|0\rangle_{q}\langle 0|+|0\rangle_{q}\langle 1| \rho|1\rangle_{q}\langle 0| & \text { if type }(q)=\text { Boolean }, \\ \sum_{n=-\infty}^{\infty}|0\rangle_{q}\langle n| \rho|n\rangle_{q}\langle 0| & \text { if type }(q)=\text { integer. }\end{cases}
$$

(UT)

$$
\overline{\langle\bar{q}:=U[\bar{q}], \rho\rangle \rightarrow\left\langle E, U \rho U^{\dagger}\right\rangle}
$$

Operational Semantics (Continued)

$$
\begin{equation*}
\frac{\left\langle S_{1}, \rho\right\rangle \rightarrow\left\langle S_{1}^{\prime}, \rho^{\prime}\right\rangle}{\left\langle S_{1} ; S_{2}, \rho\right\rangle \rightarrow\left\langle S_{1}^{\prime} ; S_{2}, \rho^{\prime}\right\rangle} \tag{SC}
\end{equation*}
$$

where $E ; S_{2}=S_{2}$.

$$
\begin{equation*}
\overline{\left\langle\mathbf{i f}\left(\square m \cdot M[\bar{q}]=m \rightarrow S_{m}\right) \mathbf{f i}, \rho\right\rangle \rightarrow\left\langle S_{m}, M_{m} \rho M_{m}^{\dagger}\right\rangle} \tag{IF}
\end{equation*}
$$

for each possible outcome $m$ of measurement $M=\left\{M_{m}\right\}$.
(L0)

$$
\overline{\langle\text { while } M[\bar{q}]=1 \text { do } S \text { od, } \rho\rangle \rightarrow\left\langle E, M_{0} \rho M_{0}^{+}\right\rangle}
$$

(L1) $\overline{\langle\text { while } M[\bar{q}]=1 \text { do } S \text { od, } \rho\rangle \rightarrow\left\langle S \text {; while } M[\bar{q}]=1 \text { do } S \text { od, } M_{1} \rho M_{1}^{+}\right\rangle}$

## Computation of a Program

Let $S$ be a quantum program and $\rho \in \mathcal{D}\left(\mathcal{H}_{\text {all }}\right)$.

1. A transition sequence of $S$ starting in $\rho$ is a finite or infinite sequence of configurations:

$$
\langle S, \rho\rangle \rightarrow\left\langle S_{1}, \rho_{1}\right\rangle \rightarrow \ldots \rightarrow\left\langle S_{n}, \rho_{n}\right\rangle \rightarrow\left\langle S_{n+1}, \rho_{n+1}\right\rangle \rightarrow \ldots
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such that $\rho_{n} \neq 0$ for all $n$ (except the last $n$ in the case of a finite sequence).

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- If a computation is finite and its last configuration is $\left\langle E, \rho^{\prime}\right\rangle$, then we say that it terminates in $\rho^{\prime}$.
- If it is infinite, then we say that it diverges.


## Outline

> Syntax

> Operational Semantics

Denotational Semantics

## Semantic Function

- If configuration $\left\langle S^{\prime}, \rho^{\prime}\right\rangle$ can be reached from $\langle S, \rho\rangle$ in $n$ steps: there are configurations $\left\langle S_{1}, \rho_{1}\right\rangle, \ldots,\left\langle S_{n-1}, \rho_{n-1}\right\rangle$ such that

$$
\langle S, \rho\rangle \rightarrow\left\langle S_{1}, \rho_{1}\right\rangle \rightarrow \ldots \rightarrow\left\langle S_{n-1}, \rho_{n-1}\right\rangle \rightarrow\left\langle S^{\prime}, \rho^{\prime}\right\rangle
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then we write:

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\langle S, \rho\rangle \rightarrow^{n}\left\langle S^{\prime}, \rho^{\prime}\right\rangle .
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- Write $\rightarrow^{*}$ for the reflexive and transitive closures of $\rightarrow$ :

$$
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if and only if $\langle S, \rho\rangle \rightarrow^{n}\left\langle S^{\prime}, \rho^{\prime}\right\rangle$ for some $n \geq 0$.

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- Let $S$ be a quantum program. Then its semantic function

$$
\begin{gathered}
\llbracket S \rrbracket: \mathcal{D}\left(\mathcal{H}_{\text {all }}\right) \rightarrow \mathcal{D}\left(\mathcal{H}_{\text {all }}\right) \\
\llbracket S \rrbracket(\rho)=\sum\left\{\left|\rho^{\prime}:\langle S, \rho\rangle \rightarrow^{*}\left\langle E, \rho^{\prime}\right\rangle\right|\right\}
\end{gathered}
$$

## Linearity

Let $\rho_{1}, \rho_{2} \in \mathcal{D}\left(\mathcal{H}_{\text {all }}\right)$ and $\lambda_{1}, \lambda_{2} \geq 0$. If $\lambda_{1} \rho_{1}+\lambda_{2} \rho_{2} \in \mathcal{D}\left(\mathcal{H}_{\text {all }}\right)$, then for any quantum program $S$ :

$$
\llbracket S \rrbracket\left(\lambda_{1} \rho_{1}+\lambda_{2} \rho_{2}\right)=\lambda_{1} \llbracket S \rrbracket\left(\rho_{1}\right)+\lambda_{2} \llbracket S \rrbracket\left(\rho_{2}\right) .
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1. An element $x \in L$ is called the least element of $L$ when $x \sqsubseteq y$ for all $y \in L$. The least element is denoted by 0 .
2. An element $x \in L$ is called an upper bound of a subset $X \subseteq L$ if $y \sqsubseteq x$ for all $x \in X$.

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- A partial order is a pair $(L, \sqsubseteq)$ where $L$ is a nonempty set and $\sqsubseteq$ is a binary relation on $L$ satisfying:

1. Reflexivity: $x \sqsubseteq x$ for all $x \in L$;
2. Antisymmetry: $x \sqsubseteq y$ and $y \sqsubseteq x$ imply $x=y$ for all $x, y \in L$;
3. Transitivity: $x \sqsubseteq y$ and $y \sqsubseteq z$ imply $x \sqsubseteq z$ for all $x, y, z \in L$.

- Let $(L, \sqsubseteq)$ be a partial order.

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- Let $(L, \sqsubseteq)$ be a CPO. Then a function $f$ from $L$ into itself is continuous if

$$
f\left(\bigsqcup_{n} x_{n}\right)=\bigsqcup_{n} f\left(x_{n}\right)
$$

for any increasing sequence $\left\{x_{n}\right\}$ in $L$.

## Knaster-Tarski Theorem

Let $(L, \sqsubseteq)$ be a CPO and function $f: L \rightarrow L$ is continuous. Then $f$ has the least fixed point

$$
\mu f=\bigsqcup_{n=0}^{\infty} f^{(n)}(0)
$$

where

$$
\begin{cases}f^{(0)}(0) & =0 \\ f^{(n+1)}(0) & =f\left(f^{(n)}(0)\right) \text { for } n \geq 0\end{cases}
$$

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- $\mathcal{E} \sqsubseteq \mathcal{F} \Leftrightarrow \mathcal{E}(\rho) \sqsubseteq \mathcal{F}(\rho)$ for all $\rho \in \mathcal{D}(\mathcal{H})$.
- $(\mathcal{Q O}(\mathcal{H}), \sqsubseteq)$ is a CPO.


## Syntactic Approximation

- abort denotes a quantum program such that

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- For any integer $k \geq 0$, the $k$ th syntactic approximation while ${ }^{(k)}$ of while:

$$
\left\{\begin{array}{rll}
\text { while }^{(0)} & \equiv \text { abort, } & \\
\text { while }^{(k+1)} & \equiv \text { if } M[\bar{q}]=0 \rightarrow \text { skip } \\
& \square & 1 \rightarrow S ; \text { while }^{(k)} \\
& \text { fi }
\end{array}\right.
$$

## Semantic Function of Loops

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\llbracket \text { while } \rrbracket=\bigsqcup_{k=0}^{\infty} \llbracket \text { while }^{(k)} \rrbracket,
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where symbol $\square$ stands for the supremum of quantum operations; i.e. the least upper bound in $\mathrm{CPO}\left(\mathcal{Q O}\left(\mathcal{H}_{\text {all }}\right), \sqsubseteq\right)$.

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Fixed Point Characterisation

For any $\rho \in \mathcal{D}\left(\mathcal{H}_{\text {all }}\right)$ :

$$
\llbracket \text { while } \rrbracket(\rho)=M_{0} \rho M_{0}^{\dagger}+\llbracket \text { while } \rrbracket\left(\llbracket S \rrbracket\left(M_{1} \rho M_{1}^{\dagger}\right)\right) .
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## Termination and Divergence Probabilities

- For any quantum program $S$ and for all partial density operators $\rho \in \mathcal{D}\left(\mathcal{H}_{\text {all }}\right):$

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- $\operatorname{tr}(\llbracket S \rrbracket(\rho))$ is the probability that program $S$ terminates when starting in state $\rho$.


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- For any finite subset $V$ of $q$ Var, for any quantum operation $\mathcal{E}$ in $\mathcal{H}_{V}$, there exists a quantum program (a block command) $S$ such that $\llbracket S \rrbracket=\mathcal{E}$.

