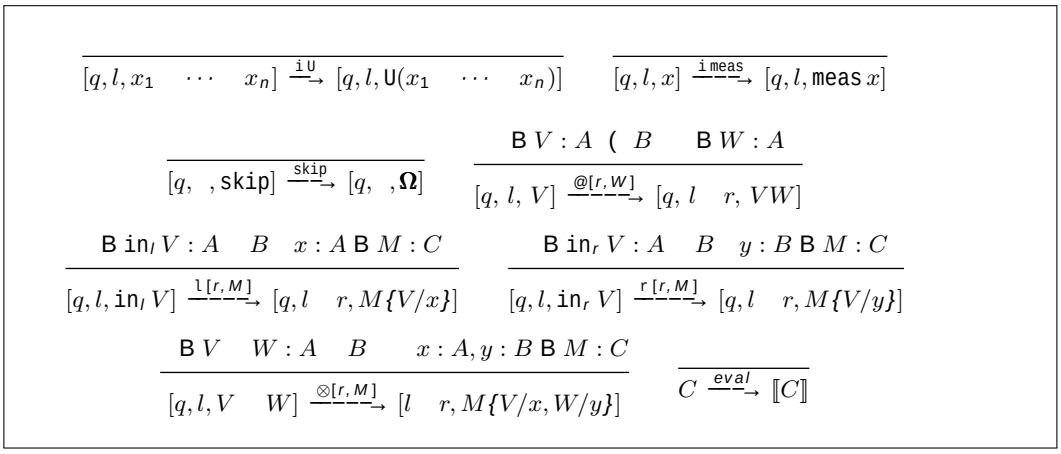

**Figure 4** Labelled Transition Rules for Quantum Closures.

## 2.3 A Probabilistic Labelled Transition System

In [14], Gordon defines explicitly a labelled transition system in order to illustrate the bisimulation technique in PCF. We follow this idea to define a *probabilistic* labelled transition system for the quantum $\lambda$-calculus, upon which we can define probabilistic bisimulations.

Transition rules are listed in Figure 4: we make the typing of terms explicit in the rules as the type system plays an important role in defining the operational semantics of typed terms. A transition takes the form $C \xrightarrow{a} \mu$, where $C$ is a quantum closure, $\mu$ is a subdistribution over quantum closures, and $a$ is an action. If $\mu$ is a point distribution $\overline{D}$, we simply write the transition as $C \xrightarrow{a} D$. Note that non-total quantum closures are needed here to specify the operational semantics: we cannot work only with total quantum closures due to entanglement. For example, we should allow for a non-total quantum closure like $[\frac{|00\rangle + |11\rangle}{\sqrt{2}}, \{x \mapsto 1\}, x]$, where the quantum variable $x$ refers to the first qubit of an entangled quantum state.

The last rule in Figure 4 says that term reductions are considered as internal transitions that are abstracted away; external transitions are labelled by *actions*. Intuitively, external transitions represent the way terms interact with environments (or contexts). For instance, a $\lambda$-abstraction can "consume" (application of itself to) a term, which is supplied by the environment as an argument, and forms a $\beta$-reduction. The rule for `skip` says that what it can provide to the environment is the value of itself, and after that it cannot provide any information, hence no external transitions can occur any more. We represent this by a transition, labelled by the value of the constant, into a non-terminating program $\mathbf{\Omega}$ of appropriate type.

The set of quantum closures $Cl$ together with the transition rules in Figure 4 yields a probabilistic labelled transition system (pLTS). It is in fact a reactive system in the sense that if $C \xrightarrow{a} \mu_1$ and $C \xrightarrow{a} \mu_2$ then $\mu_1 = \mu_2$ for all $C \in Cl$, that is no two outgoing transitions leaving a quantum closure are labelled by the same action. Below we recall Larsen and Skou's probabilistic bisimulation [22]. We first review a way of lifting a binary relation $\mathcal{R}$ over a set $S$ to be a relation $\mathcal{R}^\dagger$ over the set of subdistributions on $S$ given in [9][1].

**Definition 8.** Let $S, T$ be two countable sets and $\mathcal{R} \subseteq S \times T$ be a binary relation. The lifted relation $\mathcal{R}^\dagger \subseteq \mathcal{D}(S) \times \mathcal{D}(T)$ is defined by letting $\mu \; \mathcal{R}^\dagger \; \nu$ iff $\mu(X) \leq \nu(\mathcal{R}(X))$ for all

[1] There are several different but equivalent formulations of the lifting operation; see e.g. [27, 6].

$X \subseteq S$. Here we write $\mathcal{R}(X)$ for the set $\{t \in T \mid \exists s \in X.\ s\ \mathcal{R}\ t\}$ and $\mu(X)$ is the accumulation probability $\sum_{s \ \ X} \mu(s)$.

The definition by Larsen and Skou, when instantiated on the pLTS of closed quantum closures, looks as follows:

▮ **Definition 9.** A *probabilistic simulation* is a preorder $\mathcal{R}$ on closed quantum closures such that whenever $(C, D) \in \mathcal{R}$ we have that:

- $env(C) = env(D)$;
- $[\![C]\!]\ \mathcal{R}^{\dagger}\ [\![D]\!]$;
- if $C, D$ are values then $C \xrightarrow{a} \mu$ implies $D \xrightarrow{a} \nu$ with $\mu\ \mathcal{R}^{\dagger}\ \nu$.

A *probabilistic bisimulation* is a relation $\mathcal{R}$ such that both $\mathcal{R}$ and $\mathcal{R}^{-1}$ are probabilistic simulations. Let $\preceq$ and $\sim_s$ be the largest probabilistic simulation and bisimulation, called similarity and bisimilarity, respectively. Bisimilarity and similarity are relations on closed quantum closures, but can be generalized to open closures as follows:

Suppose $\Delta \mathsf{B} M, N : A$. We write $\emptyset \mathsf{B} M \preceq N : A$ if $[q, l, M] \preceq [q, l, N]$, and $\Delta \mathsf{B} M \sim_s N : A$ if $[q, l, M] \sim_s [q, l, N]$, for any $q$ and $l$ such that $[q, l, M]$ and $[q, l, N]$ are both typable quantum closures.

For reactive pLTSs, the kernel of probabilistic similarity is probabilistic bisimilarity. That is, $\sim_s = \preceq \cap \preceq^{-1}$. This of course also applies to the specific pLTS we are working with. The probabilistic bisimilarity defined above is a binary relation between states, and thus sometimes called state-based bisimilarity. Alternatively, it is possible to directly define a (sub)distribution-based bisimilarity by comparing actions emitted from subdistributions. In order to do so, we first define a transition relation between subdistributions.

▮ **Definition 10.** We write $\mu \xrightarrow{a} \rho$ if $\rho = \sum_{s \quad \mu} \mu(s) \cdot \mu_s$, where $\mu_s$ is determined as follows:

- either $s \xrightarrow{a} \mu_s$
- or there is no $\nu$ with $s \xrightarrow{a} \nu$, and in this case we set $\mu_s = \varepsilon$.

Note that this is a weaker notion of transition relation between subdistributions, compared with that defined on Page 432. If $\mu \xrightarrow{a} \mu$ then some (not necessarily all) states in the support of $\mu$ can perform action $a$. For example, consider the two states $s_2$ and $s_3$ in Figure 5. Since $s_2 \xrightarrow{c} \overline{s_4}$ and $s_3$ cannot perform action $c$, the distribution $\mu = \frac{1}{2}\overline{s_2} + \frac{1}{2}\overline{s_3}$ can make the transition $\mu \xrightarrow{c} \frac{1}{2}\overline{s_4}$ to reach the subdistribution $\frac{1}{2}\overline{s_4}$. Let $\mu$ be a subdistribution over a reactive pLTS. After performing any action, it can reach a unique subdistribution. That is, if $\mu \xrightarrow{a} \nu$ and $\mu \xrightarrow{a} \rho$ then $\nu = \rho$. Given a subdistribution $\mu$, we denote by $[\![\mu]\!]$ the subdistribution $\sum_{C \quad \mu} \mu(C) \cdot [\![C]\!]$.

▮ **Definition 11.** A *distribution-based bisimulation* is a binary relation $\mathcal{R}$ on subdistributions such that $\mu\ \mathcal{R}\ \nu$ implies

- $env(\mu) = env(\nu)$;
- $[\![\mu]\!]\ \mathcal{R}\ [\![\nu]\!]$;
- if $\mu$ and $\nu$ are value distributions and $\mu \xrightarrow{a} \rho$, then $\nu \xrightarrow{a} \xi$ for some $\xi$ with $\rho\ \mathcal{R}\ \xi$, and vice-versa.

Let $\sim_d$ be the largest distribution-based bisimulation. Suppose $\emptyset\ \mathsf{B}\ M, N : A$. We write $\emptyset\ \mathsf{B}\ M \sim_d N : A$ if $[\![[q, l, M]]\!] \sim_d [\![[q, l, N]]\!]$ for any $q$ and $l$ such that $[q, l, M]$ and $[q, l, N]$ are quantum closures.

It is not difficult to see that $s \sim_s t$ implies $\overline{s} \sim_d \overline{t}$ but not the other way around, as witnessed by the following example.

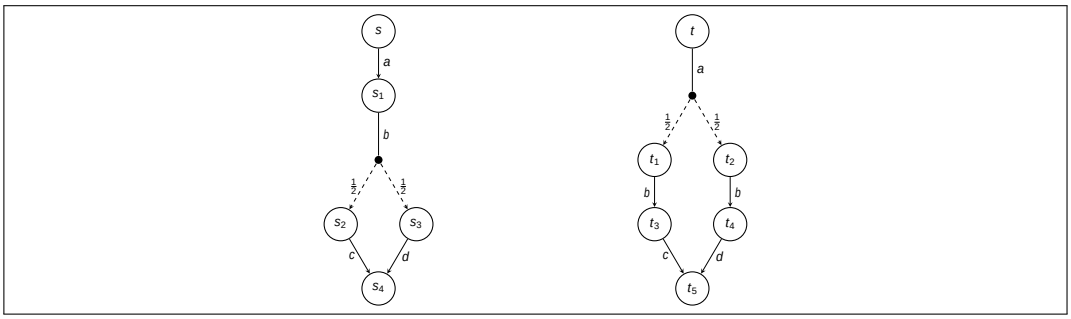


**Figure 5** $s \quad_s t$.

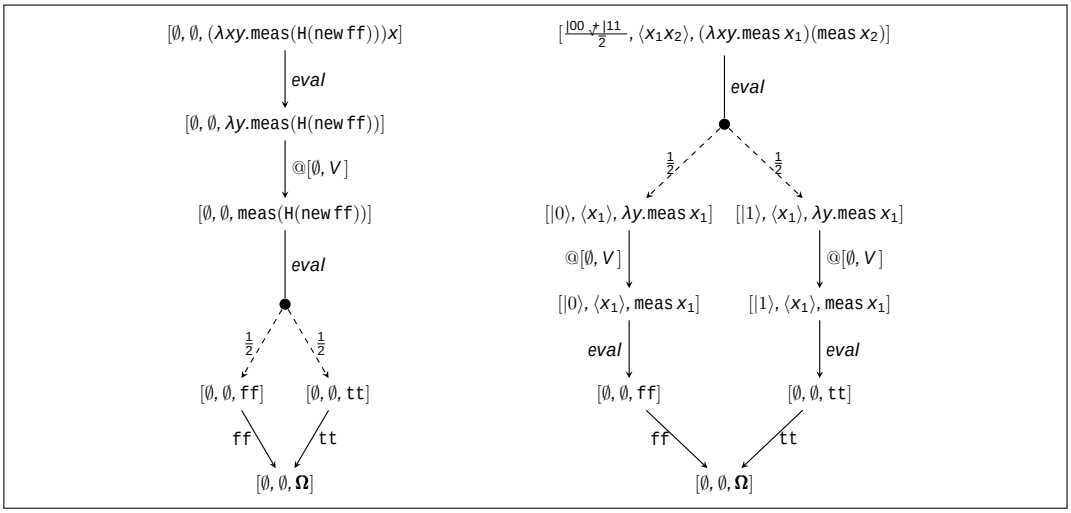


**Figure 6** Two Quantum Closures not Related by $\quad_s$.

I **Example 12.** Consider the two states $s$ and $t$ in Figure 5. We can construct the relation

$$\mathcal{R} = \{(\overline{s}, \overline{t}), \left(\overline{s_1}, \frac{1}{2}\overline{t_1} + \frac{1}{2}\overline{t_2}\right), \left(\frac{1}{2}\overline{s_2} + \frac{1}{2}\overline{s_3}, \frac{1}{2}\overline{t_3} + \frac{1}{2}\overline{t_4}\right), (\overline{s_2}, \overline{t_3}), (\overline{s_3}, \overline{t_4}), (\overline{s_4}, \overline{t_5}))\}$$

and check that $\mathcal{R}$ is a distribution-based bisimulation. Therefore, we have $\overline{s} \sim_d \overline{t}$. Note that the point distribution at state $s_1$ is related to the distribution $\frac{1}{2}\overline{t_1} + \frac{1}{2}\overline{t_2}$. However, we have $s \not\sim_s t$ because after performing action $a$ the state $s$ evolves into the point distribution $\overline{s_1}$, and the only candidate transition from $t$ to match this is $t \xrightarrow{a} \mu$ where $\mu = \frac{1}{2}\overline{t_1} + \frac{1}{2}\overline{t_2}$. But then the condition $\overline{s_1} \sim_s{}^{\dagger} \mu$ is invalid because there is no way to split $s_1$ into two different states such that they are bisimilar to $t_1$ and $t_2$ respectively. In the quantum $\lambda$-calculus this distinction between state-based and distribution-based bisimulations also exists. For example, the quantum closures $[\emptyset, \emptyset, (\lambda xy.\mathsf{meas}(\mathsf{H}(\mathsf{new}\,\mathsf{ff})))x]$ and $[\frac{|00\rangle + |11\rangle}{\sqrt{2}}, \langle x_1 x_2\rangle, (\lambda xy.\mathsf{meas}\, x_1)(\mathsf{meas}\, x_2)]$ exhibit similar behaviour as states $s$ and $t$, respectively, as depicted in Figure 6. J

## 3 Congruence

In this section we show that both $\sim_s$ and $\sim_d$ are congruence relations. The proof for $\sim_s$ is more complicated, so we take it as an example and give the details. The case for $\sim_d$ follows

$$\frac{\Delta \;\mathsf{B}\; c \quad c \quad \{x, \mathtt{skip}, \mathtt{split}^A, \mathtt{new}, \mathtt{meas}, \mathtt{U}\}}{\Delta \;\mathsf{B}\; [q,l,c] \;\hat{R}\; [q,l,c]} \qquad \frac{\Delta, x : A \;\mathsf{B}\; [q,l,M] \;\; R \;\; [r,j,N]}{\Delta \;\mathsf{B}\; [q,l,(\lambda x^A.M)] \;\hat{R}\; [r,j,(\lambda x^A.N)]}$$

$$\frac{!\Delta, \Delta' \;\mathsf{B}\; [q,l,M] \;\; R \;\; [r,j,N] \quad !\Delta, \Delta'' \;\mathsf{B}\; [q,i,L] \;\; R \;\; [r,m,P]}{!\Delta, \Delta', \Delta'' \;\mathsf{B}\; [q,l \quad i, ML] \;\hat{R}\; [r,j \quad m, NP]}$$

$$\frac{!\Delta, \Delta' \;\mathsf{B}\; [q,l,M] \;\; R \;\; [r,j,N] \quad !\Delta, \Delta'' \;\mathsf{B}\; [q,i,L] \;\; R \;\; [r,m,P]}{!\Delta, \Delta', \Delta'' \;\mathsf{B}\; [q,l \quad i, M \quad L] \;\hat{R}\; [q,j \quad m, N \quad P]}$$

$$\frac{!\Delta, \Delta' \;\mathsf{B}\; [q,l,M] \;\; R \;\; [r,j,N]}{!\Delta, \Delta' \;\mathsf{B}\; [q,l,\mathtt{in}_l\, M] \;\hat{R}\; [r,j,\mathtt{in}_l\, N]} \qquad \frac{!\Delta, \Delta' \;\mathsf{B}\; [q,l,M] \;\; R \;\; [r,j,N]}{!\Delta, \Delta' \;\mathsf{B}\; [q,l,\mathtt{in}_r\, M] \;\hat{R}\; [r,j,\mathtt{in}_r\, N]}$$

**Figure 7** Compatible Refinement Rules – Selection.

the same schema. The basic idea is to make use of Howe's method [19, 26], which requires to start from an initial relation $\mathcal{R}$, define a precongruence candidate $\mathcal{R}^H$, a precongruence relation by construction, and then to show the coincidence of that relation with the initial relation.

**Definition 13.** Let $\mathcal{R}$ be a typed relation on quantum closures. Its *compatible refinement* $\hat{\mathcal{R}}$ is defined by some natural rules, a selection of which is in Figure 7. A relation $\mathcal{R}$ is a *precongruence* iff it contains its own compatible refinement, that is $\hat{\mathcal{R}} \subseteq \mathcal{R}$. Let a *congruence* be an equivalence relation that is a precongruence.

Let $\mathcal{R}$ be a typed relation on quantum closures. The typed relation $\mathcal{R}^H$ is defined by the rules in Figure 8. Note that if $\mathcal{R}$ is reflexive then $\mathcal{R} \subseteq \mathcal{R}^H$, and $\mathcal{R}^H$ is a precongruence. Therefore, in order to show that $\mathcal{R}$ is a precongruence (or congruence if $\mathcal{R}$ is also symmetric), it suffices to establish $\mathcal{R}^H \subseteq \mathcal{R}$ because we then have the coincidence of $\mathcal{R}$ with $\mathcal{R}^H$. In order to show $(\sim_s)^H \subseteq \sim_s$, we need the following two technical lemmas.

**Lemma 14.** *If* $\emptyset \;\mathsf{B}\; [q, l, M] \preceq^H [r, j, N]$ *then* $[\![[q, l, M]]\!] \; (\preceq^H)^\dagger \; [\![[r, j, N]]\!]$. J

**Lemma 15.** *If* $\emptyset \mathsf{B} [q, l, V] \preceq^H [r, j, W]$ *then we have that* $[q, l, V] \xrightarrow{a} \mu$ *implies* $[r, j, W] \xrightarrow{a} \nu$ *and* $\mu \; (\preceq^H)^\dagger \; \nu$. J

Consequently, we can establish the coincidence of $\preceq$ with $\preceq^H$, from which it is easy to show that $\sim_s$ is a congruence. Similar arguments apply to $\sim_d$.

**Theorem 16.** *Both* $\sim_s$ *and* $\sim_d$ *are included in* $\simeq$. J

## 4 Completeness of Distribution-Based Bisimilarity

In this section we show that distribution-based bisimilarity is complete for linear contextual equivalence. The basic idea is to first characterise bisimilarity by a very simple testing framework. Let $\mathcal{T}$ be the set of tests of the two forms: $\omega$ and $a \cdot \mathtt{t}$, where $\omega$ is used to indicate success and $a$ ranges over the set of all possible labels in the transition rules in Figure 4. In other words, the testing language is given by the grammar: $\mathtt{t} ::= \omega \mid a \cdot \mathtt{t}$.

Below we define the function $Pr$ that calculates the probability of passing a test for a distribution of states in a reactive pLTS.

$$\begin{array}{rcl} Pr(\mu, \omega) & = & |\mu| \\ Pr(\mu, a \cdot \mathtt{t}) & = & Pr(\rho, \mathtt{t}) \text{ where } \mu \xrightarrow{a} \rho \end{array}$$

$$\frac{\Delta, x : A \;\mathsf{B}\; [q, l, M]\ R^H\ [r, j, N] \quad \Delta \;\mathsf{B}\; [r, j, \lambda x^A.N]\ \ R\ \ [p, i, L]}{\Delta \;\mathsf{B}\; [q, l, \lambda x^A.M]\ R^H\ [p, i, L]}$$

$$\frac{\begin{array}{c}!\Delta, \Delta' \;\mathsf{B}\; [q, l, M]\ R^H\ [r, j, N] \\ !\Delta, \Delta'' \;\mathsf{B}\; [q, i, L]\ R^H\ [r, m, P] \\ !\Delta, \Delta', \Delta'' \;\mathsf{B}\; [r, j \quad m, NP]\ \ R\ \ [s, n, Q]\end{array}}{!\Delta, \Delta', \Delta'' \;\mathsf{B}\; [q, l \quad i, ML]\ R^H\ [s, n, Q]}$$

$$\frac{\begin{array}{c}!\Delta, \Delta' \;\mathsf{B}\; [q, l, M]\ R^H\ [r, j, N] \\ !\Delta, \Delta'' \;\mathsf{B}\; [q, i, L]\ R^H\ [r, m, P] \\ !\Delta, \Delta', \Delta'' \;\mathsf{B}\; [r, j \quad m, N \quad P]\ \ R\ \ [s, n, Q]\end{array}}{!\Delta, \Delta', \Delta'' \;\mathsf{B}\; [q, l \quad i, M \quad L]\ R^H\ [s, n, Q]}$$

$$\frac{!\Delta, \Delta' \;\mathsf{B}\; [q, l, M]\ R^H\ [r, j, N] \quad !\Delta, \Delta' \;\mathsf{B}\; [r, j, \mathsf{in}_l\ N]\ R\ [p, i, L]}{!\Delta, \Delta' \;\mathsf{B}\; [q, l, \mathsf{in}_l\ M]\ R^H\ [p, i, L]}$$

$$\frac{!\Delta, \Delta' \;\mathsf{B}\; [q, l, M]\ R^H\ [r, j, N] \quad !\Delta, \Delta' \;\mathsf{B}\; [r, j, \mathsf{in}_r\ N]\ R\ [p, i, L]}{!\Delta, \Delta' \;\mathsf{B}\; [q, l, \mathsf{in}_r\ M]\ R^H\ [p, i, L]}$$

**Figure 8** Howe's Construction Rules – Selection.

If $\mu$ is a point distribution $\overline{s}$, we will write $Pr(s, t)$ for $Pr(\mu, t)$. We define a testing equivalence $=^{\mathcal{T}}$ by letting $\mu =^{\mathcal{T}} \nu$ iff $\forall t \in \mathcal{T} : Pr(\mu, t) = Pr(\nu, t)$. It turns out that the tests in $\mathcal{T}$ are sufficient to characterise $\sim_d$ as far as reactive pLTSs are concerned.

▌ **Theorem 17.** *Let $\mu$ and $\nu$ be two distributions in a reactive pLTS. Then $\mu \sim_d \nu$ if and only if $\mu =^{\mathcal{T}} \nu$.* J

Following [2], we turn each test into a corresponding context. That is, for a given test $t$ and a given type $A$, there exists a linear context $\mathcal{C}_t^A$ such that for all terms $M$ of type $A$, the success probability of $t$ applied to any total quantum closure $[q, l, M]$ is exactly the convergence probability of $[q, l, \mathcal{C}_t^A[M]]$.

▌ **Lemma 18.** *Let $A$ be a type and $t$ a test. There is a context $\mathcal{C}_t^A$ such that $\emptyset \;\mathsf{B}\; \mathcal{C}_t^A(\emptyset; A) : \mathsf{bit}$ and for every $M$ with $\emptyset \;\mathsf{B}\; M : A$, we have $Pr([q, l, M], t) = |[\![[q, l, \mathcal{C}_t^A[M]]]\!]|$, where $[q, l, M]$ and $[q, l, \mathcal{C}_t^A[M]]$ are quantum closures for any $q$ and $l$.* J

As a consequence of the previous lemma, we can show that the distribution-based bisimilarity $\sim_d$ is complete with respect to the linear contextual equivalence $\simeq$.

▌ **Theorem 19** (Full Abstraction)**.** *$\simeq$ coincides with $\sim_d$.* J

## 5 Concluding Remarks

We have presented two notions of bisimilarity for reasoning about equivalence of higher-order quantum programs in linear contexts, based on an appropriate labelled transition system for specifying the operational behaviour of programs. Both bisimilarities are sound with respect to the linear contextual equivalence, but only the distribution-based one turns out to be complete. Since linear resources are widely used in quantum computation, we believe that linear contextual equivalence will be a useful notion of behavioural equivalence for quantum

programs. The coinductive proof techniques developed in the current work can help to reason about quantum programs.

In the future, it would be interesting to seek a denotational model fully abstract with respect to the linear contextual equivalence. As recently shown in [35], Fock spaces can be useful to interpret quantum computation and they are close to the categorical semantics studied in [24], so it seems promising to start from there.

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