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Quantum weakest preconditions

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We develop a notion of predicate transformer and, in particular, the weakest precondition, appropriate for quantum computation. We show that there is a Stone-type duality between the usual state-transformer semantics and the weakest precondition semantics. Rather than trying to reduce quantum computation to probabilistic programming, we develop a notion that is directly taken from concepts used in quantum computation. The proof that weakest preconditions exist for completely positive maps follows immediately from the Kraus representation theorem. As an example, we give the semantics of Selinger's language in terms of our weakest preconditions. We also cover some specific situations and exhibit an interesting link with stabilisers.

1. Introduction

Quantum computation is rapidly becoming a significant topic in theoretical computer science. To be sure, there are still essential technological and conceptual problems to overcome in building functional quantum computers. Nevertheless, fundamental new insights have been produced into quantum computability (Deutsch 1985; Deutsch and Jozsa 1992), quantum algorithms (Grover 1996; Shor 1994) and the nature of quantum mechanics itself (Peres 1995, Part III), particularly with the emergence of quantum information theory (Nielsen and Chuang 2000, Chapter 12).

These developments inspire one to consider the problems of programming general-purpose quantum computers. Much of the theoretical research is aimed at using the new tools available – superposition, entanglement and linearity – for algorithmic efficiency. However, quantum algorithms are currently programmed at a very low level – comparable to classical computing 60 years ago. In the search for structure in the space of quantum algorithms, one is led to consider issues like compositionality, semantics, type systems and logics; these are issues that usually arise in the context of programming languages. The present paper is situated in the nascent area of quantum programming methodology and the design and semantics of quantum programming languages. We extend the well-known paradigm of *weakest preconditions* (Hoare 1969; Dijkstra 1976) to the quantum context. The influence of Dijkstra's work on weakest preconditions has been deep and pervasive, and even led to textbook level expositions of the subject (Gries 1981). The

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main point is that it leads to a *goal-directed* program, or algorithm development strategy. Hitherto, quantum algorithms have been invented by brilliant new insights. As more and more algorithms accumulate and a stock of techniques start to accumulate, a systematic program development strategy will be required. It is this that we hope will eventually come out of the present work.

In this paper we make two contributions. First, we develop the appropriate quantum analogue of weakest preconditions and develop the duality theory. Rather than reducing quantum computation to probabilistic computation and using well-known ideas from this setting (Kozen 1981; Kozen 1985), we define quantum weakest preconditions directly. It turns out that the same beautiful duality between state-transformer (forwards) and predicate-transformer (backwards) semantics that one finds in the traditional (Smyth 1983; Plotkin 1983) and probabilistic settings (Kozen 1985) appears in the quantum setting. This is related to the fact that when state transformers are specified to be completely positive maps, we can prove the existence of corresponding weakest preconditions in a very general way using a powerful mathematical result, called the Kraus representation theorem (Nielsen and Chuang 2000, Section 8.2.4). In fact, the correspondence is very much more direct in this case than in the case of conventional or probabilistic languages.

Second, we write the detailed weakest precondition semantics for a particular quantum programming language. Quantum programming languages have started to appear recently. Perhaps the best known is the quantum flow chart language (Selinger 2004), also referred to as QPL, which is based on the slogan 'quantum data and classical control'. QPL has a clean denotational semantics and a clear conceptual basis; we give an alternative weakest precondition semantics for this language. It should be noted, however, that our notion of weakest preconditions and the basic existence results are *language independent*.

The structure of this paper is as follows. In Section 2 the general setup, in particular, quantum state transformers and quantum predicates, is laid out. Next, in Section 3 we define quantum weakest preconditions and healthy predicate transformers, proving their existence for arbitrary completely positive maps and observables. In Section 4 we summarise the basic structure of Selinger's language, and develop its weakest precondition semantics. We apply our results to specific situations such as Grover's algorithm and stabilisers in Section 5, and give conclusions in Section 6.

2. The quantum framework

In this section we define the main concepts on which our theory of quantum weakest preconditions is based. We first give a general overview, after which we specify concrete definitions for quantum states and state transformers in Section 2.1 and for quantum predicates in Section 2.2.

Traditionally, there are several means of developing formal semantics for programming languages. In the operational semantics for an imperative language, one has a notion of *states*, typically denoted s, such that the commands in the language are interpreted as state transformers. If the language is deterministic, the state transformation is given by a function, and composition of commands corresponds to functional composition. The flow is forwards through the program. This type of semantics is intended to give meaning

Table 1. *Comparing situations.*

Deterministic	Probabilistic	Quantum
states s	probability distributions μ	density matrices ρ
predicates p	measurable functions f	observables M
satisfaction $s \models p$	expectation value $\int f d\mu$	quantum expectation value $\mathrm{tr}(M\rho)$

to programs that have already been written. It is useful for guiding implementations of programming languages but is, perhaps, less useful for program development. By contrast, in a predicate transformer semantics the meaning is constructed by flowing backwards through the program, starting from the final intended result and proceeding to determine what must be true of the initial input. States are replaced by *predicates* p over the state space, together with a satisfaction relation $\models$. Language constructs are interpreted as predicate transformers. This type of semantics is useful for goal-directed programming. Of course, the two types of semantics are intimately related, as they should be! In a sense to be made precise in Section 3.4, they are *dual* to each other. The situation for deterministic languages can be found in the first column of Table 1.

In the world of probabilistic programs one sees the same duality in action, after suitably generalising the notions of states and predicates. *Probability distributions* now play the role of states. There are, of course, states as before and, in a particular execution, there is only one state at every stage. However, in order to describe all the possible outcomes (and their relative probabilities), one keeps track of the probability distribution over the state space and how it changes during program execution. What plays the role of predicates? Kozen has argued (Kozen 1985) that predicates are measurable functions – or random variables, to use the probability terminology. We note that a special case of random variables are characteristic functions, which are more easily recognisable as the analogues of predicates; in fact, they *are* predicates. In a probabilistic setting one has an *expectation* value rather than truth: truth values now lie in $[0, 1]$ rather than in $\{0, 1\}$. The pairing between measurable functions f and probability distributions μ is now given by the integral, which is the probabilistic expression of the expectation value. These measurable functions are to be viewed as *observations*, which may or may not lead to termination. The pairing between f and μ then expresses the probability with which termination is achieved when observing f. The second column of Table 1 summarises the main concepts for probabilistic languages.

For the quantum world we again need a notion of state – or, more precisely, probability distributions over possible states – a notion of predicate, and a pairing. Our choices are very much guided by the probabilistic case, but we are *not* claiming that quantum computation can be seen as a special case of classical probabilistic computation. Instead, we take *density matrices* as the analogue of probability distributions, while for predicates we take the *observables* of the system. These are given by (a certain restricted class of) Hermitian operators. Finally, the notion of a pairing is again the expectation value, but given by the rules of quantum mechanics; that is, we have $\mathrm{tr}(M\rho)$, where tr stands for the usual trace from linear algebra, ρ is a density matrix and M is an observable. Throughout this paper we work with finite-dimensional Hilbert spaces, and one can think of M and ρ as matrices. We discuss these concepts in more depth in Sections 2.1 and 2.2; a summary can be found in the last column of Table 1. Note, however, that, just as for the probabilistic case, the pairing $\mathrm{tr}(M\rho)$ may be interpreted as the probability of termination when observation M is made in the state ρ.

Why can one not just use probabilistic predicates and the general theory of probabilistic predicate transformers in a quantum context? The following simple example – due to one of the referees – illustrates the reason. Suppose we have a two-dimensional Hilbert space of states with basis vectors written $|0\rangle$ and $|1\rangle$. Two other states in this Hilbert space are $\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$ and $\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)$. We use the notation $\{|\psi\rangle\}$ for the density matrix $|\psi\rangle\langle\psi|$ and write convex combinations like $\lambda\{|\psi\rangle\}+(1-\lambda)\{|\psi\rangle\}$ for the density matrix of a mixed state, that is, an ensemble. Now consider the measurable function f defined by

$$\begin{aligned} f(|0\rangle) &= 0 \\ f(|1\rangle) &= 0 \\ f\left(\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)\right) &= 1 \\ f\left(\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)\right) &= 1. \end{aligned} \tag{1}$$

This function is indeed measurable, but not linear, and cannot correspond to any kind of physical observable or measurement. To see what happens, consider the ensemble $\rho=\frac{1}{2}\{|0\rangle\}+\frac{1}{2}\{|1\rangle\}$. When f is applied to this, we get 0. However, when f is applied to the ensemble $\rho'=\frac{1}{2}\{\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)\}+\frac{1}{2}\{\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)\}$, we get the value 1. The point is that ρ and ρ' are physically indistinguishable, so one cannot have a physical observable that distinguishes between these 'two' ensembles. When developing a theory of predicates and predicate transformers we must therefore restrict ourselves to mathematical objects that are compatible with the linear structure of quantum mechanics. It is a conceptual error to think that quantum mechanics can be understood just using probabilistic constructs. We note that the work in (Butler and Hartel 1999), which uses probabilistic predicates to analyze Grover's algorithm (Grover 1996), avoids this conundrum because it considers only pure-state situations.

2.1. *Quantum states and state transformers*

Typically a quantum system is described by a Hilbert space, physical observables are described by Hermitian operators on this space and transformations of the system are effected by unitary operators (Peres 1995). However, we need to describe not only so-called *pure* states but also *mixed* states. These arise as soon as one has to deal with partial information in a quantum setting. For example, a system may be prepared as a statistical mixture, it may be mixed as a result of interactions with a noisy environment (decoherence), or by certain parts of the system being unobservable. For all these reasons we need to work with *probability distributions* over the states in a Hilbert space. In quantum mechanics this situation is characterised by *density matrices*, of which a good expository discussion appears in Nielsen and Chuang (2000, Chapter 2). Concretely, a density matrix ρ on a Hilbert space $\mathscr{H}$ is a *positive operator*, that is, for all states $|x\rangle$ in $\mathscr{H}$, we require that $\langle x|\rho x\rangle \geqslant 0$, with, furthermore, $\mathrm{tr}\rho \leqslant 1$. The reason we do not have the usual equality is that we do not assume that everything is always normalised. Hence, in order to interpret a density matrix as a probability distribution we first need to renormalise when necessary. This is a bit of a nuisance if one wants a direct interpretation of the density matrix at every stage of the computation; however, we do recover the probabilities correctly if we start with a normalised density matrix at the start of a computation and multiply out everything at the end. This convention saves some notational overhead and is used by Selinger (Selinger 2004). We denote the set of all density matrices over a Hilbert space $\mathscr{H}$ by $\mathscr{DM}(\mathscr{H})$.

As we have already mentioned, forward operational semantics is described by quantum state transformers. The properties of such state transformers are now well understood. A physical transformation must take a density matrix to a density matrix. Thus, it seems reasonable to require that physical operations correspond to positive maps, which are linear maps that take a positive operator to a positive operator. However, it is possible for a positive map to be tensored with another positive map – even an identity map – and for the result to fail to be positive. Physically this is a disaster. Indeed, this means that if we formally regard some system as part of another far away system that we do not touch (that is, to which we apply the identity transformation), then suddenly we have an unphysical transformation. A simple example is provided by the transpose operation, which is a positive map while its tensor with an identity is not. Therefore, we need the stronger requirement that physical operations are *completely* positive, a property that is defined as follows.

Definition 2.1. A map $\mathscr{E}$ is *completely positive* when it takes density matrices to density matrices, and likewise for all trivial extensions $I \otimes \mathscr{E}$.

Note that such a map may operate between distinct Hilbert spaces, that is, in general, we have $\mathscr{E} : \mathscr{DM}(\mathscr{H}_1) \to \mathscr{DM}(\mathscr{H}_2)$. We use $\mathscr{CP}(\mathscr{H}_1, \mathscr{H}_2)$ to denote the set of all such maps, and write $\mathscr{CP}(\mathscr{H})$ for $\mathscr{CP}(\mathscr{H}, \mathscr{H})$.

We frequently rely on the Kraus representation theorem for completely positive maps.

Theorem 2.1 (Kraus Theorem). The map $\mathscr{E} : \mathscr{DM}(\mathscr{H}_1) \to \mathscr{DM}(\mathscr{H}_2)$ is a completely positive map if and only if for all $\rho \in \mathscr{DM}(\mathscr{H}_1)$ we have

$$\mathscr{E}(\rho) = \sum_i E_i \rho E_i^\dagger \tag{2}$$

for some set of operators $\{E_i : \mathscr{H}_1 \to \mathscr{H}_2\}$, with $\sum_i E_i^\dagger E_i \leqslant I$.

The condition on the E_i ensures that trace of the density matrix never increases. Equation (2) is also known as the *operator-sum representation*. The proof of this theorem can be found, for example, in Nielsen and Chuang (2000, Section 8.2.4). Note there is nothing in the theorem that says that the E_i are unique.

2.2. *Quantum predicates*

In this section, we define quantum predicates and the associated order structure required for the development of our theory. Concretely, we need an ordering on predicates so that we can define *weakest* preconditions, and this order should be *Scott-continuous* in order to deal with programming language aspects such as recursion and iteration.

As argued above, quantum predicates are given by Hermitian operators. However, general Hermitian operators will not yield a satisfactory logical theory with the duality that we are looking for. We need to restrict ourselves to positive operators and, in order to obtain least upper bounds for increasing sequences, we need to bound them. More precisely, we have the following definition.

Definition 2.2. A *predicate* is a positive, and hence Hermitian, operator with the maximum eigenvalue bounded by 1.

The reason for defining predicates to have their maximum eigenvalue bounded by 1 is in order to get a complete partial order (CPO); we will clarify this below. Since our predicates are positive operators, their eigenvalues are real and positive. We denote the set of all predicates on a Hilbert space $\mathscr{H}$ by $\mathscr{P}(\mathscr{H})$.

Proposition 2.1. Let M be a Hermitian operator. Then $0 \leqslant \mathrm{tr}(M\rho) \leqslant 1$ holds for all density matrices ρ if and only if M is positive and its eigenvalues are bounded by 1.

Proof. Note that for any element $|\psi\rangle$ of $\mathscr{H}$ we have $\mathrm{tr}(M|\psi\rangle\langle\psi|) = \langle\psi \mid M \mid \psi\rangle$. Assume that $0 \leqslant \mathrm{tr}(M\rho) \leqslant 1$ for all density matrices ρ. Choose $\rho = |\psi\rangle\langle\psi|$ where $|\psi\rangle$ is an arbitrary normalised vector. We have $0 \leqslant \mathrm{tr}(M|\psi\rangle\langle\psi|) = \langle\psi \mid M \mid \psi\rangle$, which says that M is positive. Now choose $|\psi\rangle$ to be a normalised eigenvector of M with eigenvalue λ, which is necessarily real and positive, so we have $\mathrm{tr}(M|\psi\rangle\langle\psi|) = \langle\psi \mid M \mid \psi\rangle = \lambda\langle\psi|\psi\rangle = \lambda \leqslant 1$. Thus the eigenvalues are bounded by 1. The converse is obvious once we note that any density matrix is a convex combination of density matrices of the form $|\psi\rangle\langle\psi|$. □

Thus we could have defined predicates as positive operators M such that for every density matrix ρ we have $0 \leqslant \mathrm{tr}(M\rho) \leqslant 1$. This exhibits the predicates as 'dual' to density matrices.

We define an ordering as follows.

Definition 2.3. For matrices M and N in $\mathbb{C}^{n\times n}$, we define $M \sqsubseteq N$ if $N - M$ is positive.

This order is known in the literature as the *Löwner partial order* (Löwner 1934). Note that this definition can be rephrased in the following way, where $\mathscr{DM}(\mathscr{H})$ denotes the set of all density matrices.

Proposition 2.2. $M \sqsubseteq N$ if and only if $\forall\rho \in \mathscr{DM}(\mathscr{H}).\mathrm{tr}(M\rho) \leqslant \mathrm{tr}(N\rho)$

Proof. Indeed, $N - M$ positive means that for all $x \in \mathscr{H}$ we have $\langle x|N - M|x\rangle \geqslant 0$, or, equivalently, $\mathrm{tr}((N-M).|x\rangle\langle x|) \geqslant 0$. By linearity of the trace and the fact that the spectral theorem holds for all $\rho \in \mathscr{DM}(\mathscr{H})$, we get the desired result. For the converse, take all pure states $\rho = |x\rangle\langle x|$. Then we find that for all $x \in \mathscr{H}$ we have $\langle x|N - M|x\rangle \geqslant 0$, or, in other words, $M \sqsubseteq N$. □

Put another way, $M \sqsubseteq N$ if and only if the expectation value of N exceeds that of M. With the above definitions, we have the following result.

Proposition 2.3. The poset $(\mathscr{P}(\mathscr{H}), \sqsubseteq)$ is a complete partial order (CPO), that is, it contains least upper bounds of increasing sequences.

Taking predicates to be *bounded* Hermitian operators leads to Proposition 2.3, which guarantees the existence of fixpoints and thus allows for the formal treatment of iteration and recursion in Section 4.

3. Quantum weakest preconditions and duality

In this section we elaborate our theory of quantum weakest preconditions. We first give the main definitions in Section 3.1, after which we explore healthiness conditions in Section 3.2. Next, we investigate weakest precondition predicate transformers for completely positive maps in Section 3.3. With the latter results we obtain a duality between the forward state transformer semantics and the backward weakest precondition semantics in Section 3.4.

3.1. *Definitions*

In a quantum setting, the role of the satisfaction relation is taken over by the *expectation value* of an observable M, just as for probabilistic computation. The quantum expectation value of a predicate M is given by the trace expression $\mathrm{tr}(M\rho)$. Preconditions for a quantum program $\mathscr{Q}$ – described in an unspecified quantum programming language – are defined as follows. We write $\mathscr{Q}$ for the program as well as for the trace-nonincreasing completely positive map that it denotes.

Definition 3.1. The predicate M is said to be a *precondition* for the predicate N with respect to a quantum program $\mathscr{Q}$, denoted $M\{\mathscr{Q}\}N$, if

$$\forall \rho \in \mathscr{DM}(\mathscr{H}).\mathrm{tr}(M\rho) \leqslant \mathrm{tr}(N\mathscr{Q}(\rho)). \tag{3}$$

We also introduce the notation $\rho \models_r M$ to mean that $\mathrm{tr}(M\rho) \geqslant r$. Thus we think of this as a quantitative satisfaction relation with the real number r providing a 'threshold' above which we deem that ρ satisfies M.

The exact syntax of the quantum program $\mathscr{Q}$ is left unspecified deliberately, as we want to state these definitions without committing to any particular framework. Of course, we expect $\mathscr{Q}$ to implement at least some transformation on density matrices, in particular, we may think of $\mathscr{Q}$ as implementing a completely positive map. Note, however, that Definition 3.1, as well as Definition 3.2 below, does not exclude other possibilities. For example, we could also investigate possibilities proposed in Shaji and Sudarshan (2005), where it is argued that positive but not completely positive or even non-positive maps are also good candidates for describing open quantum evolutions.

This definition deserves motivation. If all density matrices were normalised, it is easy to motivate Definition 3.1: if we want the expectation value of N in the state $\mathscr{Q}(\rho)$ to be above some real number r, say, then this is guaranteed if the expectation value of M in the state ρ is above r. In the case of our unnormalised density matrices we have to do a little calculation to see that the same holds. We write the expectation value of M in a state (density matrix) ρ as $\langle M \rangle_\rho$. Now we assume that M, N and $\mathcal{Q}$ satisfy the conditions of Definition 3.1. Let ρ be any (unnormalised) density matrix, and its normalised version be $\overline{\rho} = \rho/\mathrm{tr}(\rho)$. Then we have

$$\begin{aligned}\langle M \rangle_\rho &= \mathrm{tr}(M\overline{\rho}) \\ &= \frac{1}{\mathrm{tr}(\rho)} \cdot \mathrm{tr}(M\rho) \\ &\leqslant \frac{1}{\mathrm{tr}(\rho)} \cdot \mathrm{tr}(N\mathcal{Q}(\rho)) \\ &= \frac{\mathrm{tr}(\mathcal{Q}(\rho))}{\mathrm{tr}(\rho)} \cdot \frac{1}{\mathrm{tr}(\mathcal{Q}(\rho))}\mathrm{tr}(N\mathcal{Q}(\rho)) \\ &= \frac{\mathrm{tr}(\mathcal{Q}(\rho))}{\mathrm{tr}(\rho)} \cdot \langle N \rangle_{\mathcal{Q}(\rho)} \\ &\leqslant \langle N \rangle_{\mathcal{Q}(\rho)}.\end{aligned} \tag{4}$$

Thus, even though the density matrices are not normalised and we cannot read the expectations *directly* at every intermediate stage, Definition 3.1 still has the same import as in the normalised case, as well as in the case of probabilistic predicate transformers.

From this we define weakest preconditions in the usual way.

Definition 3.2. A *weakest precondition* for a predicate M with respect to a quantum program $\mathcal{Q}$, denoted $\mathrm{wp}(\mathcal{Q})(M)$, is such that for all preconditions, $L\{\mathcal{Q}\}M$ implies $L \sqsubseteq \mathrm{wp}(\mathcal{Q})(M)$.

Note that *weakest* in this context is equal to *largest*; indeed, a larger predicate would mean that Equation (3) holds for more initial states ρ, and thus corresponds to a weaker constraint. The weakest precondition predicate transformer for a program $\mathcal{Q}$, if it exists, is denoted $\mathrm{wp}(\mathcal{Q}) : \mathcal{P}(\mathcal{H}_2) \to \mathcal{P}(\mathcal{H}_1)$, where $\mathcal{H}_2$ and $\mathcal{H}_1$ are the output and input Hilbert spaces, respectively.

3.2. *Healthiness conditions*

In analogy with Dijkstra (1976), we want to formulate *healthiness conditions* for quantum predicate transformers. These are important because they characterise exactly those programs that can be given a weakest precondition semantics that is dual to its forwards state transformer semantics. Moreover, healthiness conditions allow one to prove general laws for reasoning about programs. The healthiness conditions we propose for the quantum case are *linearity* and *complete positivity*, which lead to the following definition.

Definition 3.3. A *healthy* predicate transformer $\alpha : \mathcal{P}(\mathcal{H}_2) \to \mathcal{P}(\mathcal{H}_1)$ is a predicate transformer that is *linear* and *completely positive*, that is, it takes predicates to predicates, and similarly for all trivial extensions $I \otimes \alpha$. We use $\mathcal{PT}(\mathcal{H}_2, \mathcal{H}_1)$ to denote the associated space of healthy predicate transformers.

As we shall see in the next section, these conditions all hold in the framework where quantum programs correspond to completely positive maps. Linearity is certainly a requirement in the inherently linear context of quantum mechanics, as the example given in Section 2 clearly shows. Just as in the probabilistic case (Morgan and McIver 2004), linearity implies the analogues of some of the healthiness conditions for deterministic programs, namely feasibility, which means $\mathrm{wp}(\mathcal{Q})(0) = 0$, monotonicity and continuity. These proofs are easy and are left to the reader. The requirement that predicate transformers should be completely positive on $\mathcal{P}(\mathcal{H})$, is a very natural one. Indeed, if α is a predicate transformer, which acts only on part of a composite Hilbert space $\mathcal{H}$, then composing it with the identity predicate transformer working on the rest of the Hilbert space should still result in a valid predicate transformer.

We equip $\mathcal{PT}(\mathcal{H}_2, \mathcal{H}_1)$ with an order structure by extending the Löwner order on predicates as follows.

Definition 3.4. For healthy predicate transformers α and β in $\mathcal{PT}(\mathcal{H}_2, \mathcal{H}_1)$, we define $\alpha \sqsubseteq \beta$ if $\beta - \alpha$ is a healthy predicate transformer.

If $\alpha \sqsubseteq \beta$, then for all predicates $M \in \mathcal{P}(\mathcal{H}_2)$ we have that $\alpha(M) \sqsubseteq \beta(M)$, where $\alpha(M)$ and $\beta(M)$ are predicates on $\mathcal{H}_1$. Requiring just this would be the obvious extension of the Löwner order, but, since we are working in the space of healthy predicate transformers, we also need to demand that $\beta - \alpha$ is completely positive. That is, for all extended predicates $M_e \in \mathcal{P}(\mathcal{H}_2 \otimes \mathcal{H})$, we have $(\alpha \otimes I_{\mathcal{H}})(M_e) \sqsubseteq (\beta \otimes I_{\mathcal{H}})(M_e)$. We then have the following result.

Proposition 3.1. The poset $(\mathcal{PT}(\mathcal{H}_2, \mathcal{H}_1), \sqsubseteq)$ is a CPO.

Proof. The proof is analogous to that of Selinger (2003, Lemma 6.4). □

Note that the CPO structure as defined on predicates $\mathcal{P}(\mathcal{H})$ and associated predicate transformers $\mathcal{PT}(\mathcal{H})$ is identical to that for density matrices $\mathcal{DM}(\mathcal{H})$ and associated completely positive maps $\mathcal{CP}(\mathcal{H})$, as defined in Selinger (2003).

Furthermore, for healthy predicate transformers, we have the following immediate consequence of Kraus's theorem.

Proposition 3.2. The operator α is a healthy predicate transformer if and only if

$$\forall M \in \mathcal{P}(\mathcal{H}).\alpha(M) = \sum_u A_u^\dagger M A_u \tag{5}$$

for some set of linear operators $\{A_u\}$ such that $\sum_u A_u^\dagger A_u \leqslant I$.

3.3. *Predicate transformers for completely positive maps*

Let us now consider the following framework: the forward semantics of a quantum program $\mathcal{Q}$ is given by a trace-nonincreasing completely positive map $\mathcal{E} \in \mathcal{CP}(\mathcal{H}_1, \mathcal{H}_2)$, which we write as $[\![\mathcal{Q}]\!] = \mathcal{E}$. In this section we prove an existence theorem of weakest preconditions for completely positive maps, and show that they satisfy the healthiness conditions given in Section 3.2, that is, that they are healthy predicate transformers.

Proposition 3.3. $\forall \mathscr{E} \in \mathscr{CP}(\mathscr{H}_1, \mathscr{H}_2)$ and $N \in \mathscr{P}(\mathscr{H})$, $\mathrm{wp}(\mathscr{E})(N)$ exists and is unique. Furthermore, we have

$$\forall \rho . \mathrm{tr}(\mathrm{wp}(\mathscr{E})(N)\rho) = \mathrm{tr}(N\mathscr{E}(\rho)). \tag{6}$$

Proof. To prove existence, take an arbitrary predicate N and operation $\mathscr{E}$. From the Kraus representation theorem stated in Section 2.1,

$$\mathscr{E}(\rho) = \sum_m E_m \rho E_m^\dagger \tag{7}$$

with $\sum_m E_m^\dagger E_m \leqslant I$. Using this, together with the fact that the trace is linear and invariant under cyclic permutations, we get for a predicate N that

$$\mathrm{tr}(N\mathscr{E}(\rho)) = \mathrm{tr}((\sum_m E_m^\dagger N E_m)\rho). \tag{8}$$

If we then take

$$M = \sum_m E_m^\dagger N E_m \tag{9}$$

in Equation (8), we get

$$\forall \rho . \mathrm{tr}(M\rho) = \mathrm{tr}(N\mathscr{E}(\rho)). \tag{10}$$

So M is a precondition for N with respect to $\mathscr{E}$. Now take any other precondition M' for N with respect to $\mathscr{E}$. In other words,

$$\forall \rho . \mathrm{tr}(M'\rho) \leqslant \mathrm{tr}(N\mathscr{E}(\rho)). \tag{11}$$

However, because of Equation (10) and Proposition 2.2, this implies that $M' \sqsubseteq M$. So M is the weakest precondition for N with respect to $\mathscr{E}$, denoted $\mathrm{wp}(\mathscr{E})(N)$.

To prove uniqueness, suppose the predicate P is also a weakest precondition for N with respect to $\mathscr{E}$. Then we have $M \sqsubseteq P$, but also, since M is a weakest precondition, $P \sqsubseteq M$. But then, since $\sqsubseteq$ is an order, we have $M = P$. □

From Equation (9) and Proposition 3.2, we get the following.

Corollary 3.1. For all $\mathscr{E} \in \mathscr{CP}(\mathscr{H})$, $\mathrm{wp}(\mathscr{E}) \in \mathscr{PT}(\mathscr{H})$, that is, it is a healthy predicate transformer.

3.4. *Duality*

In this section we investigate the duality between the forward semantics of completely positive maps as state transformers and the backwards semantics of healthy predicate transformers. This duality is part of a web of dualities known to mathematicians as Stone-type dualities (Johnstone 1982), the prototype of which is the duality between boolean algebras and certain topological spaces called Stone spaces. For readers with a background in category theory we note that such a duality is captured by an adjoint equivalence mediated by a pairing, for example, the satisfaction relation between states and predicates. Kozen, following suggestions of Plotkin, found such a duality in the context of probabilistic programs (Kozen 1985). We show that such a duality also exists in the quantum setting.

In the quantum context, we find the duality by defining an isomorphism between the set of all completely positive maps $\mathscr{CP}(\mathscr{H}_1, \mathscr{H}_2)$ and the set of all healthy predicate transformers $\mathscr{PT}(\mathscr{H}_2, \mathscr{H}_1)$. We can associate a healthy predicate transformer with every operation $\mathscr{E} \in \mathscr{CP}(\mathscr{H}_1, \mathscr{H}_2)$; this follows immediately from Proposition 3.3. Indeed, we associate with every operation $\mathscr{E}$ its weakest precondition predicate transformer $\mathrm{wp}(\mathscr{E})$. To complete the duality, we need to associate an operation $\mathscr{A} \in \mathscr{CP}(\mathscr{H}_1, \mathscr{H}_2)$ with a predicate transformer $\alpha \in \mathscr{PT}(\mathscr{H}_2, \mathscr{H}_1)$. Using the operator-sum representation for predicate transformers as given in Equation (5), we have

$$\begin{aligned}\mathrm{tr}(\alpha(M)\rho) &= \mathrm{tr}\left(\left(\sum_u A_u^\dagger M A_u\right)\rho\right)\\ &= \mathrm{tr}\left(M.\left(\sum_u A_u \rho A_u^\dagger\right)\right).\end{aligned} \tag{12}$$

If we then take

$$\mathscr{A}(\rho) = \sum_u A_u \rho A_u^\dagger, \tag{13}$$

we get

$$\mathrm{tr}(\alpha(M)\rho) = \mathrm{tr}(M\mathscr{A}(\rho)), \tag{14}$$

thereby associating a state transformer with every healthy predicate transformer. Analogously to the above, one could say that this expression defines the 'strongest post-state' $\mathscr{A}(\rho)$ for a state ρ with respect to a predicate transformer $\alpha \in \mathscr{PT}(\mathscr{H})$.

To see this as a duality more clearly, we use the notation $\rho \models_r M$ defined in Section 3. Then we have

$$\frac{\mathscr{E}(\rho) \models_r M}{\rho \models_r \mathrm{wp}(\mathscr{E})M}\,. \tag{15}$$

It is straightforward to see that we have an order isomorphism between the domain of predicate transformers $\mathscr{PT}(\mathscr{H}_2, \mathscr{H}_1)$ and the domain of state transformers $\mathscr{CP}(\mathscr{H}_1, \mathscr{H}_2)$, and this for arbitrary Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$. As an aside, we observe that because of this and the fact that maps in $\mathscr{PT}(\mathscr{H}_2, \mathscr{H}_1)$ are Scott-continuous, we can immediately see that healthy predicate transformers are Scott-continuous as well.

4. Weakest precondition semantics for QPL

The quantum flow chart language or Quantum Programming Language (QPL), is a typed programming language for quantum computation with a formal semantics, which is built upon the idea of quantum data and classical control (Selinger 2004). It is very different from previously defined quantum programming languages, which do not have a formal semantics and are imperative rather than functional. Syntactically, programs in QPL are represented either by flow charts or by QPL terms. The basic language constructs are allocating or discarding bits or qubits, assignment, branching, merge, measurement and unitary transformation. One can then build more complex programs from these atomic flow chart components through context extension, vertical and horizontal composition, iteration and recursion.

At each moment, the denotation of the system, called a *state* in Selinger (2003), is given by a tuple of density matrices. The tuple dimension originates from classical bits present in the program, while tuple entries represent the state of all available qubits as density matrices. Each member of the tuple corresponds to a particular instantiation of the classical variables in lexicographical order; this is otherwise interpreted as a classical control path. Concretely, a state for a typing context containing n bits and m qubits is given by a 2^n-tuple $(\rho_0, \ldots, \rho_{2^n-1})$ of density matrices in $\mathscr{DM}(\mathbb{C}^{2^m})$. Program transformations are given by tuples of trace-decreasing completely positive maps that act on states – these are called superoperators in Selinger (2003). Note that positivity on tuples is defined so that it holds for each entry, while the trace of a tuple is defined as the sum of the traces of its entries.

The formal semantics of QPL is developed within the category **Q**, which has signatures (which define tuples of complex finite-dimensional vector spaces) as its objects and superoperators as its morphisms. This category is equipped with a CPO-structure, composition, a coproduct $\oplus$ and a tensor product $\otimes$, all of which are Scott-continuous, and a monoidal trace **Tr**. The latter is just the categorical trace for the co-pairing map $\oplus$; as in Selinger (2003), we use the term monoidal to avoid confusion with the categorical trace for the tensor product, that is, the matrix trace tr. The coproduct $\oplus$ denotes concatenation of signatures. Note that, unlike the very similar situation for finite-dimensional vector spaces, it is *not* a product, as the diagonal map $\Delta : A \rightarrow A \oplus A$ does not respect matrix traces and hence is not a superoperator. All basic flow chart components are morphisms of this category. For example, the semantics of the measurement of one qubit q is defined as

$$[\![\text{measure } q]\!] : \mathbf{qbit} \rightarrow \mathbf{qbit} \oplus \mathbf{qbit} : \rho \rightarrow (\mathscr{E}_0 \oplus \mathscr{E}_1)(\rho) = P_0 \rho P_0 \oplus P_1 \rho P_1, \tag{16}$$

where $P_\psi = |\psi\rangle\langle\psi|$. Context extension is modelled by specific $\oplus$ or $\otimes$ operations on the state. Vertical and horizontal composition correspond to composition and coproducts of morphisms, respectively, while iteration is interpreted via the monoidal trace. Specifically, suppose that an operation $\mathscr{E} : \sigma \oplus \tau \rightarrow \sigma' \oplus \tau$, where σ, σ' and τ are signatures, has been decomposed into components $\mathscr{E}_{11} : \sigma \rightarrow \sigma'$, $\mathscr{E}_{12} : \sigma \rightarrow \tau$, $\mathscr{E}_{21} : \tau \rightarrow \sigma'$ and $\mathscr{E}_{22} : \tau \rightarrow \tau$. The operation obtained from $\mathscr{E}$ by iterating over τ is then given by the *monoidal trace of* $\mathscr{E}$, defined by

$$\mathbf{Tr}(\mathscr{E}) = \mathscr{E}_{11} + \sum_{i=0}^{\infty} \mathscr{E}_{21} ; \mathscr{E}_{22}^{i} ; \mathscr{E}_{12}. \tag{17}$$

The CPO structure on superoperators (Selinger 2003) ensures the existence of this limit.

QPL also allows recursively defined operations $\mathscr{E} = F(\mathscr{E})$, where F is a flow chart. In this case, F defines a Scott-continuous function Φ_F on morphisms such that the interpretation of $\mathscr{E}$ is given as the least fixed point of Φ_F. Concretely,

$$\mathscr{E} = \sqcup_i F_i \qquad \text{with } F_0 = 0 \text{ and } F_{i+1} = \Phi_F(F_i) \tag{18}$$

$$= \sqcup_i \Phi_F^i(0), \tag{19}$$

where 0 is the zero completely positive map, which corresponds to the divergent program. Again, the existence of these fixed points is ensured by the CPO structure.

In the following, we derive a weakest precondition semantics for QPL. Note that in order to to this, our predicates need to operate on tuples of density matrices. We do this by writing expressions of the type $M_1 \oplus M_2$, where M_1 and M_2 are predicates in the sense of Definition 2.2. This works since $\oplus$ is in fact defined on arbitrary linear maps. We frequently write $\mathrm{wp}(\mathscr{Q})$ instead of $\mathrm{wp}([\![\mathscr{Q}]\!])$; by which we mean that we use the forward semantics of $\mathscr{Q}$, which is given by a tuple of completely positive maps, to derive the weakest precondition predicate transformer for $\mathscr{Q}$ according to the results in Section 3.3.

Basic flow charts In our approach we uniformly consider all basic flow charts to be operations in the operator-sum representation as in Equation (7). As such, Proposition 3.3 already provides a weakest precondition semantics for these atomic flow charts. Note, however, that predicates need to be defined in accordance with the type of the tuple exiting a basic flow chart. As a concrete example, we mention measurement, for which the forward semantics is specified in Equation (16). We find that for all predicates $M_1 \oplus M_2$ we have

$$\begin{aligned} \mathrm{wp}(\textbf{measure } q)(M_1 \oplus M_2) &= \mathrm{wp}(\mathscr{E}_0 \oplus \mathscr{E}_1)(M_1 \oplus M_2) \\ &= \mathrm{wp}(\mathscr{E}_0)(M_1) + \mathrm{wp}(\mathscr{E}_1)(M_2) \\ &= P_0 M_1 P_0 + P_1 M_2 P_1. \end{aligned} \tag{20}$$

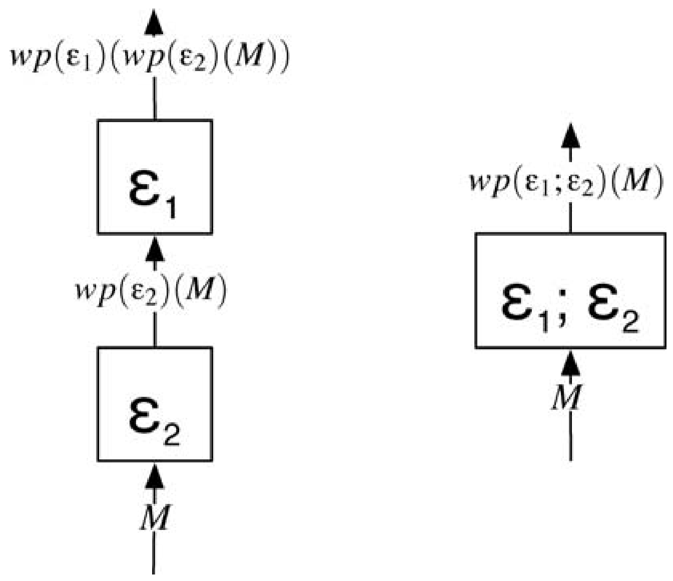
We now turn towards weakest precondition relations for composition techniques of QPL.

Sequential composition Suppose we take the sequential composition of two operations $\mathscr{E}_1$ and $\mathscr{E}_2$, as shown in Figure 1. For the composed operation $\mathscr{E}_1;\mathscr{E}_2$ and for all predicates M we have

$$\mathrm{tr}(M.(\mathscr{E}_1;\mathscr{E}_2)(\rho)) = \mathrm{tr}(\mathrm{wp}(\mathscr{E}_1;\mathscr{E}_2)(M).\rho). \tag{21}$$

If we calculate weakest preconditions for both operations separately and then compose them sequentially, we get

$$\begin{aligned} \mathrm{tr}(M.(\mathscr{E}_1;\mathscr{E}_2)(\rho)) &= \mathrm{tr}(M.\mathscr{E}_2(\mathscr{E}_1(\rho))) \\ &= \mathrm{tr}(\mathrm{wp}(\mathscr{E}_2)(M).\mathscr{E}_1(\rho)) \\ &= \mathrm{tr}(\mathrm{wp}(\mathscr{E}_1)(\mathrm{wp}(\mathscr{E}_2)(M)).\rho) \\ &= \mathrm{tr}((\mathrm{wp}(\mathscr{E}_2);\mathrm{wp}(\mathscr{E}_1))(M).\rho). \end{aligned} \tag{22}$$



$wp(\varepsilon_1)(wp(\varepsilon_2)(M))$
ε_1
$wp(\varepsilon_2)(M)$
ε_2
M
$wp(\varepsilon_1;\varepsilon_2)(M)$
$\varepsilon_1;\ \varepsilon_2$
M

Fig. 1. Sequential composition schematically.

Hence, by Equations (21) and (22), we get that weakest predicate transformers compose sequentially as follows,

$$\mathrm{wp}(\mathscr{E}_1;\mathscr{E}_2) = \mathrm{wp}(\mathscr{E}_2);\mathrm{wp}(\mathscr{E}_1). \tag{23}$$

This is the same rule as found for sequential composition in classical programming languages (Dijkstra 1976).

Parallel composition Suppose we take the parallel composition of two operations $\mathscr{E}_1$ and $\mathscr{E}_2$, as shown in Figure 2. For the composed operation $\mathscr{E}_1 \oplus \mathscr{E}_2$ we have

$$\mathrm{tr}((M_1 \oplus M_2).(\mathscr{E}_1 \oplus \mathscr{E}_2)(\rho_1 \oplus \rho_2)) = \mathrm{tr}(\mathrm{wp}(\mathscr{E}_1 \oplus \mathscr{E}_2)(M_1 \oplus M_2).(\rho_1 \oplus \rho_2)). \tag{24}$$

On the other hand, if we calculate weakest preconditions for both operations separately and then compose them in a parallel way, we get

$$\begin{aligned}\mathrm{tr}((M_1 \oplus M_2).(\mathscr{E}_1 \oplus \mathscr{E}_2)(\rho_1 \oplus \rho_2)) &= \mathrm{tr}(M_1.\mathscr{E}_1(\rho_1) \oplus M_2.\mathscr{E}_2(\rho_2))\\ &= \mathrm{tr}(M_1.\mathscr{E}_1(\rho_1)) + \mathrm{tr}(M_2.\mathscr{E}_2(\rho_2))\\ &= \mathrm{tr}(\mathrm{wp}(\mathscr{E}_1)(M_1).\rho_1) + \mathrm{tr}(\mathrm{wp}(\mathscr{E}_2)(M_2).\rho_2)\\ &= \mathrm{tr}((\mathrm{wp}(\mathscr{E}_1)(M_1) \oplus \mathrm{wp}(\mathscr{E}_2)(M_2)).(\rho_1 \oplus \rho_2))\\ &= \mathrm{tr}((\mathrm{wp}(\mathscr{E}_1) \oplus \mathrm{wp}(\mathscr{E}_2))(M_1 \oplus M_2).(\rho_1 \oplus \rho_2)).\end{aligned} \tag{25}$$

Comparing Equations (24) and (25), we get that for parallel composition weakest precondition predicate transformers compose as follows,

$$\mathrm{wp}(\mathscr{E}_1 \oplus \mathscr{E}_2) = \mathrm{wp}(\mathscr{E}_1) \oplus \mathrm{wp}(\mathscr{E}_2) \tag{26}$$

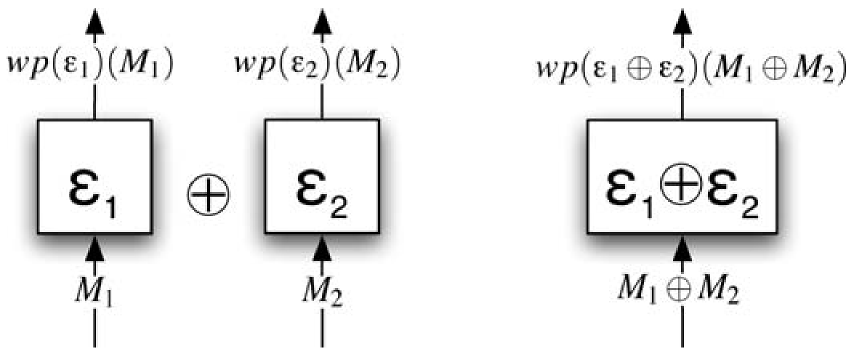


Fig. 2. Parallel composition schematically.

Context extension We will now look at what happens if we weaken a context with dummy classical or quantum variables. Suppose first that we have a QPL program $\mathcal{Q}$ with denotation $\mathcal{E}$. We first modify $\mathcal{Q}$ by picking a fresh classical variable b and adding it to $\mathcal{Q}$'s context; we denote the resulting program $\mathcal{Q}_b$. The forward semantics of the latter is given by $\mathcal{E} \oplus \mathcal{E}$ (Selinger 2004), and hence by Equation (26), we find that

$$\mathrm{wp}(\mathcal{Q}_b) = \mathrm{wp}(\mathcal{Q}) \oplus \mathrm{wp}(\mathcal{Q}). \tag{27}$$

Suppose next that we add a fresh qubit q to $\mathcal{Q}$'s context, and write $\mathcal{Q}_q$ for the resulting program. The forward semantics of $\mathcal{Q}_q$ is given by

$$[\![\mathcal{Q}_q]\!]\left(\begin{array}{c|c} \rho_1 & \rho_2 \\ \hline \rho_3 & \rho_4 \end{array}\right) = \left(\begin{array}{c|c} \mathcal{E}(\rho_1) & \mathcal{E}(\rho_2) \\ \hline \mathcal{E}(\rho_3) & \mathcal{E}(\rho_4) \end{array}\right), \tag{28}$$

which we write more concisely as

$$[\![\mathcal{Q}_q]\!] = \left(\begin{array}{c|c} \mathcal{E} & \mathcal{E} \\ \hline \mathcal{E} & \mathcal{E} \end{array}\right). \tag{29}$$

Accordingly, we find that

$$\mathrm{wp}(\mathcal{Q}_q) = \left(\begin{array}{c|c} \mathrm{wp}(\mathcal{E}) & \mathrm{wp}(\mathcal{E}) \\ \hline \mathrm{wp}(\mathcal{E}) & \mathrm{wp}(\mathcal{E}) \end{array}\right). \tag{30}$$

Iteration Consider a flow chart that is obtained from a program $\mathcal{Q}$ by introducing a loop, as shown in Figure 3. As explained in the above, the semantics of the flow chart is given by the monoidal trace $\mathbf{Tr}(\mathcal{E})$, where $\mathcal{E}$ is the semantics of the flow chart obtained from $\mathcal{Q}$ by removing the loop. For a predicate M we have

$$\mathrm{tr}(M.(\mathbf{Tr}(\mathcal{E}))(\rho)) = \mathrm{tr}(\mathrm{wp}(\mathbf{Tr}(\mathcal{E}))(M).\rho). \tag{31}$$

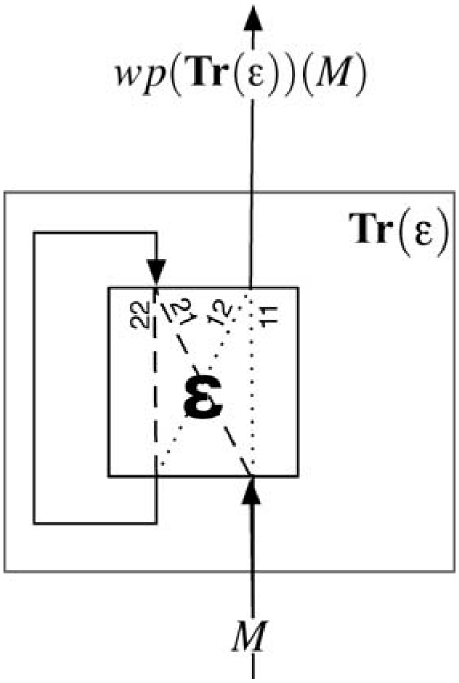


Fig. 3. Iteration schematically.

By iterating explicitly and using Equations (17) and (23), we get

$$\begin{aligned}
&\operatorname{tr}(M.(\mathbf{Tr}(\mathscr{E}))(\rho)) \\
&= \operatorname{tr}\left(M.\left(\mathscr{E}_{11} + \sum_{i=0}^{\infty} \mathscr{E}_{21}; \mathscr{E}_{22}^{i}; \mathscr{E}_{12}\right)(\rho)\right) \\
&= \operatorname{tr}(M.\mathscr{E}_{11}(\rho)) + \sum_{i=0}^{\infty} \operatorname{tr}(M.(\mathscr{E}_{21}; \mathscr{E}_{22}^{i}; \mathscr{E}_{12})(\rho)) \\
&= \operatorname{tr}(\mathrm{wp}(\mathscr{E}_{11})(M).\rho) + \sum_{i=0}^{\infty} \operatorname{tr}((\mathrm{wp}(\mathscr{E}_{12}); \mathrm{wp}(\mathscr{E}_{22})^{i}; \mathrm{wp}(\mathscr{E}_{21}))(M).\rho) \\
&= \operatorname{tr}\left(\left(\mathrm{wp}(\mathscr{E}_{11}) + \sum_{i=0}^{\infty} \mathrm{wp}(\mathscr{E}_{12}); \mathrm{wp}(\mathscr{E}_{22})^{i}; \mathrm{wp}(\mathscr{E}_{21})\right)(M).\rho\right).
\end{aligned} \tag{32}$$

Comparing Equations (31) and (32), we get

$$\mathrm{wp}(\mathbf{Tr}(\mathscr{E})) = \mathrm{wp}(\mathscr{E}_{11}) + \sum_{i=0}^{\infty} \mathrm{wp}(\mathscr{E}_{12}); \mathrm{wp}(\mathscr{E}_{22})^{i}; \mathrm{wp}(\mathscr{E}_{21}). \tag{33}$$

Moreover, the existence of the limit in Equation (33) is guaranteed by Proposition 3.1.

Recursion Consider an operation that is defined recursively, that is, an operation $\mathscr{E}$ satisfying the equation $\mathscr{E} = F(\mathscr{E})$, where F is a flow chart. The required fixed point solution to this recursive equation is given by Equations (18) and (19). If we work out the weakest precondition relations using Equation (18) and the fact that weakest precondition predicate transformers are Scott-continuous, we get

$$\begin{aligned}\mathrm{tr}(M.\mathscr{E}(\rho)) &= \mathrm{tr}(M.(\sqcup_i F_i)(\rho)) \\ &= \mathrm{tr}(\mathrm{wp}(\sqcup_i F_i)(M).\rho) \\ &= \mathrm{tr}((\sqcup_i \mathrm{wp}(F_i))(M).\rho).\end{aligned} \tag{34}$$

Combining this result with Proposition 3.3, we find that the weakest precondition predicate transformer for a recursively defined operation $\mathscr{E} = F(\mathscr{E})$ is obtained as

$$\mathrm{wp}(\mathscr{E}) = \sqcup_i \mathrm{wp}(F_i) = \sqcup_i \mathrm{wp}(\Phi_F^i(0)). \tag{35}$$

The existence of the least upper bound in Equation (35) is guaranteed by Proposition 3.1. Of course, this result depends on the concrete recursive specification considered. Specifically, one needs to determine Φ_F in order to determine the weakest precondition predicate transformer corresponding to an operation $\mathscr{E}$, defined recursively as $\mathscr{E} = F(\mathscr{E})$.

5. Applications

In this section we look at some specific situations and their weakest precondition predicate transformers.

5.1. *Grover's algorithm*

We first look into Grover's algorithm, also known as the database search algorithm (Grover 1996). The algorithm is parameterised by the number of qubits n and is specified in QPL as follows, where we write N for 2^n:

```
Grover(N) ::= new qint_n q := $\frac{1}{\sqrt{N}}\sum_{i=0}^{N-1}|i\rangle$;
              new int k := C;
              while k > 0 do {                                   (36)
                  q *= G;
                  k := k − 1;
              }
              measure q
```

Note that we assume the presence of product types of quantum integers $qint_n$ – qubit registers of size n – and integers int, which were elaborated in Selinger (2003), and also the presence of integer operations.

The Grover operator G is given by

$$G = O;IAM, \tag{37}$$

where O is a quantum oracle, which labels solutions to the search problem, and IAM is the *inversion about mean* operation, specifically, $IAM = \frac{2}{N}\sum_{i,j=0}^{N-1}|i\rangle\langle j| - I$.

Supposing the solution to the search problem is given by s, the relevant postcondition for Grover is given by $\bigoplus_{i=0}^{N-1} |s\rangle\langle s|$; in particular, we want to get

$$\mathrm{tr}\left(\bigoplus_{i=0}^{N-1} |s\rangle\langle s|\rho_{f_i}\right) = 1, \tag{38}$$

where $\bigoplus_{i=0}^{N-1} \rho_{f_i}$ is the final state of the algorithm, and the tuple summation is present because of measurement branching.

We work our way backwards through the algorithm using Equation (23) in order to find the weakest precondition corresponding to the postcondition $\bigoplus_{i=0}^{N-1} |s\rangle\langle s|$. First we derive the weakest precondition for the measurement in the last step of the algorithm. We do this according to a generalisation of Equation (20) for N-valued measurements, as follows:

$$\begin{aligned} \mathrm{wp}(\textbf{measure}\ q)\left(\bigoplus_{i=0}^{N-1} |s\rangle\langle s|\right) &= \mathrm{wp}(\mathscr{E}_0 \oplus \ldots \oplus \mathscr{E}_{N-1})\left(\bigoplus_{i=0}^{N-1} |s\rangle\langle s|\right) \\ &= \mathrm{wp}(\mathscr{E}_0)(|s\rangle\langle s|) + \cdots + \mathrm{wp}(\mathscr{E}_{N-1})(|s\rangle\langle s|) \\ &= P_0|s\rangle\langle s|P_0 + \cdots + P_{N-1}|s\rangle\langle s|P_{N-1} \\ &= |s\rangle\langle s|. \end{aligned} \tag{39}$$

Note that, since the remainder of the algorithm consists of unitary evolution, all relevant preconditions continue to be pure state projectors. In this case, Equation (38) holds only if the output state equals the predicate, that is, if $\rho_f = |s\rangle\langle s|$, so that pure state preconditions are also the states required for the algorithm to satisfy Equation (38) after termination.

We now focus on the while loop in the algorithm. Geometrically, the Grover operator is a rotation in the two-dimensional space (Nielsen and Chuang 2000, Section 6.1.3) spanned by the states $|s\rangle$ and

$$|\alpha\rangle = \frac{1}{\sqrt{N-1}} \sum_{x \neq s} |x\rangle. \tag{40}$$

More specifically, G can be decomposed as

$$G = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \quad \text{with } \sin\theta = \frac{2\sqrt{N-1}}{N}. \tag{41}$$

Applying Equation (23) again, we get the following as weakest precondition with respect to the while loop:

$$\mathrm{wp}(\textbf{while}\ \ k > 0\ \ \textbf{do}\ q \mathrel{*}= G)(|s\rangle\langle s|) = (G^C)^\dagger|s\rangle\langle s|G^C, \tag{42}$$

where we omit explicit weakest precondition reasoning for the purely classical command $k := k - 1$. Using Equation (41), we see that $(G^C)^\dagger|s\rangle$ corresponds to C rotations over an angle of $-\theta$ in the state space spanned by $|\alpha\rangle$ and $|s\rangle$. By choosing $C = \arccos\frac{1}{\sqrt{N}}$ (Nielsen and Chuang 2000, Section 6.1.3), we rotate the postcondition $|s\rangle\langle s|$ towards the precondition $|\psi_i\rangle\langle\psi_i|$, where $|\psi_i\rangle$ is the initial state of the algorithm, that is, the equal superposition state, which lies in the space spanned by the states $|\alpha\rangle$ and $|s\rangle$. In other words, using Equation (6) and Equation (38), we get that for all ρ_i

$$\begin{aligned} \operatorname{tr}(\mathrm{wp}(\mathit{Grover})(|s\rangle\langle s|)\rho_i) &= \operatorname{tr}(|s\rangle\langle s|\mathit{Grover}(\rho_i)) \\ \iff \operatorname{tr}(|\psi_i\rangle\langle\psi_i|\rho_i) &= 1. \end{aligned} \tag{43}$$

That is, Equation (38) holds if and only if $\rho_i = |\psi_i\rangle\langle\psi_i|$, which is the case by construction of the algorithm. Hence we have established the correctness of the algorithm via our backwards semantics.

Note that an alternative derivation for Grover's algorithm based on probabilistic weakest preconditions has been reported in Butler and Hartel (1999). However, the use of probabilistic notions only works there because Grover's algorithm is considered for pure states only. The mathematical structures underlying their analysis is that of probabilistic weakest preconditions, which are, in fact, not at all suited to a generalised quantum setting, as we have stressed in Section 2. In our setting we could reason about mixed state solutions to Grover and compare them with the pure state solution elaborated in the above. Also, while it may seem at first sight that the value of C in Butler and Hartel (1999) is derived via the backward semantics, this is in fact not the case. Instead, a recurrence relation for amplitudes occurring in each Grover iteration is solved; these amplitudes are found by applying the Grover iteration backwards, just as we did. We chose to adhere to the interpretation of G as a rotation in a two-dimensional state space in order to find C; we could just as well have adhered to the derivation in Butler and Hartel (1999). While their proof is an ingenious alternative to that in Nielsen and Chuang (2000), it is not based on the theory of probabilistic weakest preconditions.

5.2. *Tossing a coin*

As a second application, we derive the weakest precondition for the flow chart implementing a fair coin toss (Selinger 2004, Example 4.1). In QPL terms, the flow chart is specified as follows, where r is an input qubit register of unspecified length:

$$\begin{aligned} \mathit{coin}(r) ::= {} & \textbf{new qbit } q := \mathbf{0}; \\ & q \mathrel{*}= H; \\ & \textbf{measure } q; \\ & \textbf{discard } q \end{aligned} \tag{44}$$

An arbitrary postcondition for this program is of the form $M_1 \oplus M_2$, where M_1 and M_2 are both predicates over $\mathscr{P}(\mathbb{C}^{2^n})$ and n is the number of qubits in the register r. We derive the corresponding weakest precondition by flowing backwards through the program, starting with the discard operation. The latter induces the following quantum operation, where I_N is the $(N \times N)$ identity map with $N = 2^n$ as before, 0 denotes the $(N \times N)$ zero block matrix, and ρ is a density matrix in $\mathscr{DM}(\mathbb{C}^{2^{n+1}})$:

$$[\![\textbf{discard } q]\!](\rho) = \begin{pmatrix} I_N \,|\, 0 \end{pmatrix} \rho \begin{pmatrix} I_N \\ \hline 0 \end{pmatrix} + \begin{pmatrix} 0 \,|\, I_N \end{pmatrix} \rho \begin{pmatrix} 0 \\ \hline I_N \end{pmatrix}. \tag{45}$$

This leads to the following weakest precondition:

$$\mathrm{wp}(\textbf{discard}\ q)(M_1 \oplus M_2) = \left(\begin{array}{c|c} M_1 & 0 \\ \hline 0 & M_1 \end{array}\right) \oplus \left(\begin{array}{c|c} M_2 & 0 \\ \hline 0 & M_2 \end{array}\right). \tag{46}$$

Next, we have the measurement step. We just give the result here, as this type of derivation has already been covered in the Grover example above:

$$\mathrm{wp}(\textbf{measure}\ q)\left[\left(\begin{array}{c|c} M_1 & 0 \\ \hline 0 & M_1 \end{array}\right) \oplus \left(\begin{array}{c|c} M_2 & 0 \\ \hline 0 & M_2 \end{array}\right)\right] = \left(\begin{array}{c|c} M_1 & 0 \\ \hline 0 & M_2 \end{array}\right). \tag{47}$$

The Hadamard transformation is straightforward and leads to

$$\mathrm{wp}(q \mathrel{*}= H)\left(\begin{array}{c|c} M_1 & 0 \\ \hline 0 & M_2 \end{array}\right) = \frac{1}{2}\left(\begin{array}{c|c} M_1 + M_2 & M_1 + M_2 \\ \hline M_1 + M_2 & M_1 + M_2 \end{array}\right). \tag{48}$$

Finally, we move through the first command in the coin toss program, namely the addition of a new qubit. The forward semantics of this command is as follows, where ρ is a density matrix in $\mathscr{DM}(\mathbb{C}^{2^n})$:

$$[\![\textbf{new qbit}\ q := \mathbf{0}]\!](\rho) = \left(\begin{array}{c} I_N \\ \hline 0 \end{array}\right) \rho \left(\begin{array}{c|c} I_N & 0 \end{array}\right). \tag{49}$$

Hence, we get

$$\mathrm{wp}(\textbf{new qbit}\ q := \mathbf{0})\left(\frac{1}{2}\left(\begin{array}{c|c} M_1 + M_2 & M_1 + M_2 \\ \hline M_1 + M_2 & M_1 + M_2 \end{array}\right)\right) = \frac{1}{2}(M_1 + M_2). \tag{50}$$

Wrapping all individual steps of the coin toss program up into one weakest precondition predicate transformation according to Equation (23), we get

$$\mathrm{wp}(\mathit{coin}(r))(M_1 \oplus M_2) = \frac{1}{2}(M_1 + M_2). \tag{51}$$

5.3. *Stabilisers are predicates*

The stabiliser formalism is an alternative description of quantum states (Gottesman 1999). Instead of describing states as vectors in a suitable Hilbert space, they are described by a set of operators that leave the state invariant. Concretely, for an n-qubit system these operators are taken from the Pauli group G_n, that is, the group of n-fold tensor products of the Pauli matrices with factors $\pm 1, \pm i$ in front. Note that if we allow all positive operators instead, we get the more familiar density matrix formalism. Of course not all states can be described in this way. Formally, a *stabiliser state* is a simultaneous eigenvector of an abelian subgroup of the Pauli group with eigenvalue 1. This subgroup is then called the *stabiliser* S of this state, and usually represented by its generators. Surprisingly, some forms of entanglement, such as graph states (Raussendorf *et al.* 2003), for example, as well as all Clifford group operations, can be described efficiently via stabilisers – a celebrated result known as the *Gottesman–Knill theorem* (Nielsen and Chuang 2000, Section 10.5.4). This is because the stabiliser S for an n-qubit stabiliser state has $n-1$ generators (as opposed to 2^n amplitudes in the state formalism). A nice overview of stabiliser theory can be found in Nielsen and Chuang (2000, Chapter 10).

Stabilisers, which are unitaries, fit well within the setting of weakest preconditions, because when restricting ourselves to pure states, they *are*, in fact, quantum predicates. This follows from the following theorem.

Proposition 5.1. Given a pure state $\rho = |\psi\rangle\langle\psi|$ and a unitary U, we have

$$\mathrm{tr}(U\rho) = 1 \iff U|\psi\rangle = |\psi\rangle. \tag{52}$$

Proof. For the left to right direction, we have

$$\begin{aligned}
&\mathrm{tr}(U|\psi\rangle\langle\psi|) = \langle\psi \mid U \mid \psi\rangle = 1\\
&\Rightarrow (\langle\psi| - \langle\psi|U^\dagger)(|\psi\rangle - U|\psi\rangle) = 0\\
&\Rightarrow |\psi\rangle - U|\psi\rangle = 0\\
&\Rightarrow |\psi\rangle = U|\psi\rangle.
\end{aligned} \tag{53}$$

The other direction is obvious. □

For example, consider the creation of a Bell state

$$|B\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

by applying $U = CNOT.(H \otimes I)$ to $|00\rangle$. The stabiliser of $|B\rangle$ is generated by Z_1Z_2 and X_1X_2. Hence, by the above result, we have $\mathrm{tr}(Z_1Z_2\mathscr{E}_U(|\psi\rangle\langle\psi|)) = \mathrm{tr}(X_1X_2\mathscr{E}_U(|\psi\rangle\langle\psi|)) = 1$, where $|\psi\rangle$ is the initial state of the algorithm and $\mathscr{E}_U(\rho) = U\rho U^\dagger$ for all ρ. Applying Equation (9), we get as weakest preconditions $\mathrm{wp}(\mathscr{E}_U)(Z_1Z_2) = Z_2$ and $\mathrm{wp}(\mathscr{E}_U)(X_1X_2) = Z_1$. So, by Proposition 3.3, we also have $\mathrm{tr}(Z_1|\psi\rangle\langle\psi|) = \mathrm{tr}(Z_2|\psi\rangle\langle\psi|) = 1$. But then, by the above result, Z_1 and Z_2 are stabilisers of $|\psi\rangle$. Hence $|\psi\rangle = |00\rangle$, as required.

6. Conclusions

In this article, we have developed the predicate transformer and weakest precondition formalism for quantum computation. We did this by first noting that the quantum analogue to predicates are expectation values of quantum measurements, given by the expression $\mathrm{tr}(M\rho)$. Then we defined the concept of weakest preconditions within this framework, proving that a weakest precondition exists for arbitrary completely positive maps and observables. We have also worked out the weakest precondition semantics for the Quantum Programming Language (QPL) developed in Selinger (2003). QPL is the first model for quantum computation with a denotational semantics, and as such the first serious attempt to design a quantum programming language intended for programming quantum algorithms compositionally.

With this development in place one can envisage a goal-directed programming methodology for quantum computation. Of course one needs more experience with quantum programming idioms, and the field is not yet ready to produce a 'quantum' Science of Programming. It is likely that in the field of communication protocols, such as those based on teleportation, we have a good stock of ideas and examples that could be used as the basis of methodologies in this context.

The most closely related work, apart from Selinger's work on his programming language, is the work by Sanders and Zuliani (Sanders and Zuliani 2000), which develops a guarded command language used for developing quantum algorithms. This is a very interesting paper and works seriously towards developing a methodology for quantum algorithms. However, they use probability and nondeterminism to capture probabilistic aspects of quantum algorithms. Ours is an *intrinsically quantum* framework. The notion of weakest precondition that we develop here is not related to anything in their framework. There is other, as yet unpublished, work (Baltag and Smets 2006) in which a quantum dynamic logic is being developed. Clearly, such work will be related though they use a different notion of pairing. Also, the work in Edalat (2004) is related and merits further investigation. Edalat uses the interval domain of reals, rather than the reals, as the values of the entries in his density matrices. This seems a good way to deal with uncertainty in the values.

There is a large literature on probabilistic predicate transformers, including several papers from the probabilistic systems group at Oxford. A forthcoming book (Morgan and McIver 2004) gives an expository account of their work. We emphasise again that the theory of probabilistic predicate transformers does not capture the proper notions appropriate for the quantum setting. Linearity and complete positivity are essential aspects of the theory of quantum predicate transformers. If one tries to work with probabilistic predicates alone, one will not be able to express healthiness conditions that capture the physically allowable transformations, as the example presented in Section 3 illustrates.

One might worry that the predicates are too restricted. There are many 'observables' in physics that are not positive; for example, the z-component of angular momentum, written J_z, for a spin $\frac{1}{2}$ system takes on the values $\pm\frac{1}{2}$. However, for reasoning about the evolution of J_z one can work instead with the operator $\frac{1}{2}[I + J_z]$, which has eigenvalues $\frac{1}{4}$ and $\frac{3}{4}$, and so is a predicate. Of course one cannot do this for unbounded operators like the energy, but this will not be a handicap for quantum computation.

One pleasant aspect of the present work is that it is language independent; though we have used it to give the semantics of QPL, the weakest precondition formalism stands on its own. We can therefore apply it to other computational models that are appearing, for example, the one-way model (Raussendorf and Briegel 2001; Raussendorf *et al.* 2003), for which language ideas are just emerging (Danos *et al.* 2004).

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References

Beltag, A. and Smets, S. (2006) LQP: The dynamic logic of quantum information. *Mathematical Structures in Computer Science* **16** (3) 491–525.

Butler, M.J. and Hartel, P.H. (1999) Reasoning about Grover's quantum search algorithm using probabilistic wp. *ACM transactions on programming languages and systems* **21** (3) 417–430.

Danos, V., Kashefi, E. and Panangaden, P. (2004) The measurement calculus. quant-ph/0412135.

Deutsch, D. (1985) Quantum theory, the Church–Turing principle and the universal quantum computer. *Proc. R. Soc. Lond.* **A400** 97–117.

Deutsch, D. and Jozsa, R. (1992) Rapid solution of problems by quantum computation. *Proc. R. Soc. Lond.* **A** 439–553.

Dijkstra, E.W. (1976) *A Discipline of Programming*, Prentice-Hall.

Edalat, A. (2004) An extension of Gleason's theorem for quantum computation. *Int. J. of Theor. Phys.* (to appear).

Gottesman, D. (1999) The Heisenberg representation of quantum computers. In: Corney, S.P., Delbourgo, R. and Jarvis, P.D. (eds.) *Proceedings of the XXII International Colloquium on Group Theoretical Methods in Physics*, International Press 32–43.

Gries, D. (1981) *The Science of Programming*, Springer-Verlag.

Grover, L.K. (1996) A fast quantum mechanical algorithm for database search. In: *ACM Symposium on Theory of Computing* 212–219.

Hoare, C. (1969) An axiomatic basis for computer programming. *Communications of the ACM* **12** (10) 576–580.

Johnstone, P. (1982) *Stone Spaces*, Cambridge Studies in Advanced Mathematics **3**, Cambridge University Press.

Kozen, D. (1981) Semantics of probabilistic programs. *Journal of Computer and Systems Sciences* **22** 328–350.

Kozen, D. (1985) A probabilistic PDL. *Journal of Computer and Systems Sciences* **30** (2) 162–178.

Löwner, K. (1934) Uber monotone matrixfunktionen. *Mathematische Zeitschrift* **38** 177–216.

Morgan, C. and McIver, A. (2004) *Abstraction, refinement and proof for probabilistic systems*, Springer-Verlag.

Nielsen, M.A. and Chuang, I. (2000) *Quantum computation and quantum information*, Cambridge University Press.

Peres, A. (1995) *Quantum Theory: Concepts and Methods*, Kluwer Academic Publishers.

Plotkin, G.D. (1983) Lecture notes on domain theory.

Raussendorf, R. and Briegel, H.J. (2001) A one-way quantum computer. *Phys. Rev. Lett.* **86** (22) 5188–5191.

Raussendorf, R., Browne, D.E. and Briegel, H.J. (2003) Measurement-based quantum computation on cluster states. *Phys. Rev. A* **68** (2) 022312.

Sanders, J.W. and Zuliani, P. (2000) Quantum programming. In: Mathematics of Program Construction. *Springer-Verlag Lecture Notes in Computer Science* **1837** 80–99.

Selinger, P. (2004) Towards a quantum programming language. *Mathematical Structures in Computer Science* **14** 527–586.

Shaji, A. and Sudarshan, E. (2005) Who's afraid of not completely positive maps? *Phys. Lett. A* **341** 48–54.

Shor, P.W. (1994) Algorithms for quantum computation: Discrete logarithms and factoring. In: *IEEE Symposium on Foundations of Computer Science* 124–134.

Smyth, M. (1983) Powerdomains and predicate transformers. In: Diaz, J. (ed.) Proceedings of the International Colloquium On Automata Languages And Programming. *Springer-Verlag Lecture Notes in Computer Science* **154** 662–676.