An Algebraic Method to Fidelity-based Model Checking over Quantum Markov Chains

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Abstract

Fidelity is one of the most widely used quantities in quantum information that measure the distance of quantum states through a noisy channel. In this paper, we introduce a quantum analogy of computation tree logic (CTL) called QCTL, which concerns fidelity instead of probability in probabilistic CTL, over quantum Markov chains (QMCs). Noisy channels are modelled by super-operators, which are specified by QCTL formulas; the initial quantum states are modelled by density operators, which are left parametric in the given QMC. The problem is to compute the minimum fidelity over all initial states for conservation. We achieve it by a reduction to quantifier elimination in the existential theory of the reals. The method is absolutely exact, so that QCTL formulas are proven to be decidable in exponential time. Finally, we implement the proposed method and demonstrate its effectiveness via a quantum IPv4 protocol.

Keywords: Model Checking, Formal Logic, Quantum Computation, Computer Algebra

1. Introduction

Markov chains (MCs) have attracted a lot of attention in the field of formal verification [7, 8]. In 1989, Hansson and Jonsson introduced probabilistic computation tree logic (PCTL) to specify quantitative properties over MCs, and presented an algorithm to check whether a property \( \phi \) holds over a MC \( \mathcal{M} \) [20]. The complexity is polynomial time w.r.t. the size of both \( \phi \) and \( \mathcal{M} \). Later, more efficient approximation algorithms were presented and implemented in various model checkers, such as PRISM [23], iscasMC [18] and Storm [9], to solve numerous practical problems. Such model checkers provide a Boolean answer to the decision problem: either \( \mathcal{M} \) satisfies \( \phi \) or not. In case of a negative answer, a counter-example can further be provided [19] to locate the potential bug. Thereby, the model checking technology has achieved great success in both academic and industrial communities.

Quantum hardware has been rapidly developed in the last decades, particularly in very recent years. For example, in October 2019 Google officially announced that its 53-qubit Sycamore processor took about 200 seconds to sample one instance of a quantum circuit that would have taken the world’s most powerful supercomputer 10,000 years [3]. People tend to believe that special-purpose quantum computers with more than 100 qubits will be available in nearly 5 years. In
the meantime, quantum software will be crucial in harnessing the power of quantum computers, such as the BB84 protocol for quantum key distribution [6], Shor’s algorithm for integer factorization [26], Grover’s algorithm for unstructured search [16], and the HHL algorithm for solving linear equations [21]. To ensure the reliability of quantum software, verification technologies are urgent to be developed for quantum systems and protocols. Due to the features in quantum mechanics, three major challenges in verification are:

1. the state space is a continuum,
2. quantum information cannot be cloned [28], and
3. measurement destroys quantum information.

To tackle them effectively, researchers had to impose restrictions on the quantum model. Gay et al. [14, 15] restricted the quantum operations to the Clifford group gates (including Hadamard, CNOT and phase gates), restricted the state space to a set of finitely describable states called stabilizers that is closed under those Clifford group gates, and applied PRISM to check the quantum protocols—superdense coding, quantum teleportation, and quantum error correction. Whereas, Feng et al. proposed the model of super-operator weighted Markov chain [12], which gave rise to an alternative way to finitely describable states. The model was shown to be able to describe some hybrid systems [24]. Under the model, the authors considered the reachability probability [31], the repeated reachability probability [11], and the model checking of linear time properties [24] and a quantum analogy of computation tree logic (QCTL) [12]. A key step in their work is decomposing the state space (known as a Hilbert space) into a direct-sum of some bottom strongly connected component (BSCC) subspaces plus a maximal transient subspace w.r.t. a given super-operator. After decomposition, all the aforementioned problems were shown to be computable/decidable in polynomial time.

The above works studied only the probability measure of some properties, which is characterized by the trace of the final partial density operator. Specifically, suppose a quantum system is in the state \( \rho \) and some quantum channel \( \mathcal{E} \) occurs, changing the quantum system to the state \( \mathcal{E}(\rho) \). The probability measure concerns merely \( \text{tr}(\rho) \) and \( \text{tr}(\mathcal{E}(\rho)) \), which are abstractions on the whole \( \rho \) and \( \mathcal{E}(\rho) \). For instance, the quantum states \( \rho = |0\rangle\langle 0| \) and \( \mathcal{E}(\rho) = |1\rangle\langle 1| \) (where \( \mathcal{E} \) is the bit flip) have the same probability/trace 1, but they are entirely different. In other words, we fail to detect the effect of the bit flip channel. The reason is that, in the abstraction from \( \rho \) to \( \text{tr}(\rho) \), a lot of information concerning the quantum state is lost. In the occasions of reasoning about noisy channels, this is far from being satisfactory. The current work proposes to use fidelity in place of probability measure to specify the properties of quantum Markov chains. Fidelity is a basic concept in quantum information that prescribes the quantification of the similarity degree of two quantum states. As a measure for the distance between the quantum states \( \rho \) and \( \mathcal{E}(\rho) \), the fidelity, ranging in \([0, 1]\), characterizes precisely how well a quantum channel \( \mathcal{E} \) could preserve the information of the quantum system. Qualitatively, the fidelity is nonnegative, vanishes if and only if \( \rho \) and \( \mathcal{E}(\rho) \) have support on mutually orthogonal subspaces, and attains its maximum value 1 if and only if the two states are identical. It decreases as two states become more distinguishable, where the distinguishability reflects the effect of a quantum channel. For instance, the fidelity between \( |0\rangle\langle 0| \) and \( |1\rangle\langle 1| \) reaches the minimum 0 as expected. Hence the probability measure does not suffice to recognize general quantum states, but the fidelity does!

In this paper, we consider the fidelity-based property over (super-operator weighted) quantum Markov chains (QMCs). This property is specified by another quantum analogy of computation tree logic (QCTL), including a novel kind of fidelity-quantifier formula instead of the trace-quantifier formula in [12]. Since the state formulas and the path formulas in QCTL are mutually
inductive, we perform the model checking in three steps: i) decide the basic state formulas, ii) synthesize the super-operators of path formulas, and iii) decide the fidelity-quantifier formulas. The last step plays a central role in the model checking, and depends on the second step. To solve it, we first remove the BSCC subspaces that cover all fixed-points of a super-operator in consideration. By Brouwer’s fixed-point theorem, the direct-sum of all these BSCC subspaces are easily obtained. Then we explicitly express the super-operators using matrix representation. Finally the fidelity-quantifier formula is decided by a reduction to quantifier elimination in the existential theory of the reals. The complexity is shown to i) be exponential time for the QMC with a parametric initial quantum state; and ii), as an immediate corollary, be polynomial time for the QMC with a concrete initial quantum state. As a running example, the quantum IPv4 protocol is checked to demonstrate the effectiveness of the proposed method.

Finally, we summarize the contributions of the paper as follows:

1. a useful fidelity-based QCTL is presented;
2. all BSCC subspaces are removed by their direct-sum, not individual ones, which makes our process more efficient than the existing work [11];
3. the complexity is compatible/competitive when the QMC is provided with an initial quantum state, e.g. in [30].

Organization of the paper. Section 2 gives the basic notions and notations from quantum computation. Sections 3 and 4 introduce the model of QMC and the logic of QCTL, respectively. Section 5 presents the model checking algorithm, incorporating with an algebraic approach to the fidelity computation. Section 6 is the conclusion.

2. Preliminaries

Here we recall some basic notions and notations in quantum computation. Interested readers can refer to [23,12] for more details.

In this paper, we adopt the Dirac notations:

- $\lvert \psi \rangle$ stands for a unit column vector labelled with $\psi$;
- $\langle \psi \rvert := \lvert \psi \rangle^\dagger$ is the Hermitian adjoint (i.e. complex conjugate and transpose) of $\lvert \psi \rangle$;
- $\langle \psi_1 \vert \psi_2 \rangle := \langle \psi_1 \rvert \langle \psi_2 \rangle$ is the inner product of $\lvert \psi_1 \rangle$ and $\lvert \psi_2 \rangle$; and
- $\lvert \psi_1 \rangle \langle \psi_2 \rvert := \lvert \psi_1 \rangle \otimes \langle \psi_2 \rangle$ is the outer product, where $\otimes$ denotes tensor product.

Specifically, $\lvert i \rangle$ with $i \in \mathbb{Z}^+$ denotes the vector, in which the $i$th entry is 1 and others are 0. Thus, $\langle i \vert j \rangle = 0$ holds for any positive integer $j \neq i$ by orthonormality.

Let $[n]$ ($n \in \mathbb{Z}^+$) denote the finite set $\{1,2,\ldots,n\}$. Let $\mathcal{H}$ be a Hilbert space with dimension $d := \dim(\mathcal{H})$ throughout this paper. Unit elements $\lvert \psi \rangle$ of $\mathcal{H}$ are usually interpreted as states of a quantum system. Since $\{\lvert i \rangle : i \in [d]\}$ forms an orthonormal basis of $\mathcal{H}$, any element $\lvert \psi \rangle$ of $\mathcal{H}$ can be expressed as $\lvert \psi \rangle = \sum_{i \in [d]} c_i \lvert i \rangle$, where $c_i \in \mathbb{C}$ (i.e. complex numbers) satisfy $\sum_{i \in [d]} |c_i|^2 = 1$, i.e. the quantum state $\lvert \psi \rangle$ is entirely determined by those coefficients $c_i$. In a product Hilbert space $\mathcal{H} \otimes \mathcal{H}'$, let $\lvert \psi, \psi' \rangle$ be a shorthand of the product state $\lvert \psi \rangle \lvert \psi' \rangle := \lvert \psi \rangle \otimes \lvert \psi' \rangle$ with $\lvert \psi \rangle \in \mathcal{H}$ and $\lvert \psi' \rangle \in \mathcal{H}'$. For any $\lvert \psi_1 \rangle, \lvert \psi_2 \rangle \in \mathcal{H}$ and $\lvert \psi'_1 \rangle, \lvert \psi'_2 \rangle \in \mathcal{H}'$, the inner product of two product states $\lvert \psi_1, \psi'_1 \rangle$ and $\lvert \psi_2, \psi'_2 \rangle$ is defined by $\langle \psi_1, \psi'_1 \vert \psi_2, \psi'_2 \rangle = \langle \psi_1 \rvert \psi_2 \rangle \langle \psi'_1 \rvert \psi'_2 \rangle$. 

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Let $\mathcal{L}_H$ be the set of linear operators on $\mathcal{H}$, ranged over by letters in bold font, e.g. $E, F, I, P$. For conciseness, we will omit such a subscript $\mathcal{H}$ afterwards if it is clear from the context. A linear operator $\gamma$ is Hermitian if $\gamma = \gamma^\dagger$; and it is positive if $\langle \psi | \gamma | \psi \rangle \geq 0$ holds for any $|\psi\rangle \in \mathcal{H}$.

Given a Hermitian operator $\gamma$, we have the spectral decomposition \cite[Box 2.2]{Bo04} that

$$\gamma = \sum_{i \in [d]} \lambda_i |\psi_i\rangle\langle\psi_i|,$$

(1)

where $\lambda_i \in \mathbb{R}$ ($i \in [d]$) are all eigenvalues of $\gamma$ and $|\psi_i\rangle$ are the corresponding eigenvectors. The support of $\gamma$ is the subspace of $\mathcal{H}$ spanned by all eigenvectors associated with nonzero eigenvalues, i.e. 

$$\text{supp}(\gamma) := \text{span}(|\psi_i\rangle : i \in [d] \land \lambda_i \neq 0) = \{ \sum_{i \in [d]} c_i |\psi_i\rangle : c_i \in \mathbb{C} \land \lambda_i \neq 0 \}.$$ 

A projector $P$ is a positive operator of the form $\sum_{i \in [m]} |\psi_i\rangle\langle\psi_i|$ with $m \leq d$, where $|\psi_i\rangle$ ($i \in [m]$) are orthonormal. Obviously, there is a bijective map between projectors $P = \sum_{i \in [m]} |\psi_i\rangle\langle\psi_i|$ and subspaces of $\mathcal{H}$ that are spanned by $\{|\psi_i\rangle : i \in [m] \}$.

In sum, positive operators are Hermitian ones whose eigenvalues are nonnegative; and projectors are positive operators whose eigenvalues are 0 or 1.

The trace of a linear operator $\gamma$ is defined as $\text{tr}(\gamma) := \sum_{i \in [d]} |\langle \psi_i | \gamma | \psi_i \rangle|$ for any orthonormal basis $\{|\psi_i\rangle : i \in [d] \}$ of $\mathcal{H}$. A density operator (resp. partial density operator) $\rho$ on $\mathcal{H}$ is a positive operator with trace 1 (resp. $\leq 1$). It gives rise to a generic way to describe quantum states: if a density operator $\rho$ is $|\psi\rangle\langle\psi|$ for some $|\psi\rangle \in \mathcal{H}$, $\rho$ is said to be a pure state; otherwise it is a mixed one, i.e. $\rho = \sum_{i \in [d]} p_i |\psi_i\rangle\langle\psi_i|$ under the spectral decomposition, where $p_i$ ($i \in [d]$) are positive probabilities (interpreted as the probabilities of taking the pure states $|\psi_i\rangle$) and together are 1.

Sometimes, the quantum states are described by the probabilistic ensemble form $\langle (p_i, |\psi_i\rangle) : i \in [d] \rangle$ with $|\psi_i\rangle \in \mathcal{H}$ and $p_i \in \mathbb{R}^+$ satisfying $\sum_{i \in [d]} p_i = 1$. Note that the probabilistic ensemble form does not require that $|\psi_i\rangle$ ($i \in [d]$) are orthogonal, so it is more general. Let $D$ be the set of positive operators on $\mathcal{H}$, and $D^1$ the set of density operators. In a product Hilbert space $\mathcal{H} \otimes \mathcal{H}'$, $\gamma \otimes \gamma'$ with $\gamma \in \mathcal{L}_H$ and $\gamma' \in \mathcal{L}_{H'}$ has the partial traces $\text{tr}_H(\gamma \otimes \gamma') := \text{tr}(\gamma')\gamma$ and $\text{tr}_{H'}(\gamma \otimes \gamma') := \text{tr}(\gamma)\gamma'$, which result in linear operators in $\mathcal{H}$ and $\mathcal{H}'$, respectively. The (partial) trace is defined to be linear in its input.

A super-operator $E$ on $\mathcal{H}$ is a linear operator on $\mathcal{L}_H$, ranged over by letters in calligraphic font, e.g. $E, F, I, P$. A super-operator is completely positive if for any Hilbert space $\mathcal{H}'$, the trivially extended operator $E \otimes I_{\mathcal{H}'}$ maps the set of positive operators on $\mathcal{L}_{\mathcal{H}'\otimes\mathcal{H}}$ to itself, where $I_{\mathcal{H}'}$ is the identity super-operator on $\mathcal{H}'$. Let $S$ be the set of completely positive super-operators on $\mathcal{H}$. By Kraus representation \cite[Thm. 8.3]{Kra71}, a super-operator $E$ is completely positive on $\mathcal{H}$ if and only if there are $m$ linear operators $E_1, E_2, \ldots, E_m \in L$ with $m \leq d^2$ (called Kraus operators), such that for any $\gamma \in S$, we have

$$E(\gamma) = \sum_{\ell \in [m]} E_\ell \gamma E^\dagger_\ell.$$ 

(2)

The description of $E$ is given by those Kraus operators $\{E_\ell : \ell \in [m]\}$. Thus, the sum $E_1 + E_2$ of super-operators $E_1 = \{E_{1,\ell} : \ell \in [m_1]\}$ and $E_2 = \{E_{2,\ell} : \ell \in [m_2]\}$ is given by the union $\{E_{1,\ell} : \ell \in [m_1]\} \cup \{E_{2,\ell} : \ell \in [m_2]\}$; and the composition $E_2 \circ E_1$ is given by $\{E_{2,\ell} : \ell \in [m_1]\} \circ \{E_{1,\ell} : \ell \in [m_2]\} = \{E_{2,\ell} \circ E_{1,\ell} : \ell \in [m_1] \land \ell_2 \in [m_2]\}$.

In a product Hilbert space $\mathcal{H} \otimes \mathcal{H}'$, for super-operators $E = \{E_\ell : \ell \in [m]\} \in S_{\mathcal{H} \otimes \mathcal{H}'}$, the product super-operator $E \otimes E'$ is given by $\{E_{\ell,\ell'} : \ell \in [m] \land \ell' \in [m']\} = \{E_{\ell} \otimes E'_{\ell'} : \ell \in [m] \land \ell' \in [m']\}$. It is easy to validate that $E \otimes E'(\gamma \otimes \gamma') = E(\gamma) \otimes E'(\gamma')$ holds for any $\gamma \in \mathcal{L}_H$ and $\gamma' \in \mathcal{L}_{H'}$.

For a super-operator $E \in S$ and a density operator $\rho \in D^1$, the fidelity is defined as

$$\text{Fid}(E, \rho) := \frac{1}{4} \text{tr} \left( \rho^{1/2} E(\rho) \rho^{1/2} \right);$$

(3a)
and when $\rho$ is a pure state $|\psi\rangle\langle\psi|$, it is simply

$$\text{Fid}(E, |\psi\rangle\langle\psi|) := \sqrt{\langle\psi| E(|\psi\rangle\langle\psi|) |\psi\rangle}.$$  \hfill (3b)

The fidelity reflects how well the quantum operation $E$ has preserved the quantum state $\rho$. The better quantum state is preserved, the larger fidelity would be. We can see $0 \leq \text{Fid}(E, \rho) \leq 1$ where the equality in the first inequality holds if and only if the supports of $\rho$ and $E(\rho)$ are orthogonal, and the equality in the second inequality holds if and only if $E = I$. More technically, the fidelity measures the average angle between the vectors in $\text{supp}(\rho)$ and those in $\text{supp}(E(\rho))$, which reveals that $\arccos \text{Fid}(E, \rho)$ would be a standard metric between $\rho$ and $E(\rho)$. For conservation, we would like to study the (minimum) fidelity of $E$, which is defined as

$$\text{Fid}(E) := \min_{\rho \in \mathcal{D}} \text{Fid}(E, \rho) = \min_{|\psi\rangle \in \mathcal{H}} \text{Fid}(E, |\psi\rangle\langle\psi|),$$  \hfill (3c)

where the last equation comes from the joint concavity [25, Ex. 9.19].

A trace pre-order $\lesssim$ can be defined on $S$ as: $\mathcal{E}_1 \lesssim \mathcal{E}_2$ if and only if $\text{tr}(\mathcal{E}_1(\rho)) \leq \text{tr}(\mathcal{E}_2(\rho))$ holds for any $\rho \in \mathcal{D}$. The equivalence $\mathcal{E}_1 \simeq \mathcal{E}_2$ means $\mathcal{E}_1 \lesssim \mathcal{E}_2$ and $\mathcal{E}_1 \gtrless \mathcal{E}_2$. For a super-operator $E = \{E_t : t \in [m]\}$, the completeness $E \simeq I$ holds if and only if $\Sigma_{t \in [m]} E_t^{\dagger} E_t = I$ where $I$ is the identity operator. Let $S^{\lesssim I}$ be the set of trace-nonincreasing super-operators $E$, i.e. $S^{\lesssim I} = \{E \in S : \mathcal{E} \lesssim I\}$. We would characterize quantum state evolution by these super-operators $E \in S^{\lesssim I}$ in the coming section.

3. Quantum Markov Chain

Let $AP$ be a set of atomic propositions throughout this paper.

**Definition 3.1 ([12, Def. 3.1]).** A labelled quantum Markov chain (QMC for short) $\mathcal{C}$ over $\mathcal{H}$ is a triple $(S, Q, L)$, in which

- $S$ is a finite set of states,
- $Q : S \times S \rightarrow S^{\lesssim I}$ is a transition super-operator matrix, satisfying $\Sigma_{s \in S} Q(s, t) = I$ for each $s \in S$, and
- $L : S \rightarrow 2^{AP}$ is a labelling function.

Let $|s\rangle$ ($s \in S$) be the quantisation of classical state $s$, and $\{|s\rangle : s \in S\}$ a set of orthonormal states serving as the quantisation of classical system $S$. Once all classical states in $S$ are ordered, $|s\rangle$ denotes the $|s|$-dimensional vector, in which the entry corresponding to $s$ is 1 and others are 0. Further, $\mathcal{H}_{eq} := C \otimes \mathcal{H}$ where $C = \text{span}(|s\rangle : s \in S)$ is the enlarged Hilbert space corresponding to the whole classical–quantum system. The dimension of $\mathcal{H}_{eq}$ is $N := nd$ where $n = |S|$. In the QMC $\mathcal{C}$, a state $\rho$ is given by a density operator on $\mathcal{H}_{eq}$ with the mixed structure $\Sigma_{s \in S} |s\rangle\langle s| \otimes \rho_s$ where $\rho_s \in \mathcal{D}$ ($s \in S$) satisfy $\Sigma_{s \in S} \text{tr}(\rho_s) = 1$. The initial state is left parametric in the model.

The transition super-operator matrix $Q$ is functionally analogous to the transition probability matrix in an ordinary Markov chain (MC). Actually, the former is more expressive than the latter, and a QMC degenerates into an MC when $\mathcal{H}$ is one-dimensional. Sometimes, it is convenient to combine the super-operators in $Q$ together to form a large single super-operator, denoted $\mathcal{F} := \Sigma_{s \in S} |s\rangle\langle s| \otimes Q(s, t)$, on $\mathcal{H}_{eq}$. 

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A path \( \omega \) in the QMC \( \mathcal{C} \) is an infinite state sequence in the form \( s_0 \ s_1 \ s_2 \ldots \), where \( s_i \in S \) and \( Q(s_i, s_{i+1}) \neq 0 \) for \( i \geq 0 \). Let \( \omega(i) \) be the \((i+1)\)-th state of \( \omega \) for \( i \geq 0 \), e.g. \( \omega(0) = s_0 \) and \( \omega(1) = s_1 \) for \( \omega = s_0 \ s_1 \ s_2 \ldots \). We denote by \( \text{Path}(s) \) the set of all paths starting in \( s \), and by \( \text{Path}_{in}(s) \) the set of all finite paths starting in \( s \), i.e. \( \text{Path}_{in}(s) := \{ \tilde{\omega} : \tilde{\omega} \text{ is a finite prefix of some } \omega \in \text{Path}(s) \} \).

**Example 3.2 (IPv4 protocol).** The IPv4 protocol \([1]\) aims at configuring IP addresses in a LAN of hosts. A quantum analogy goes as follows. When a new host joins in a LAN, it gets an IP address at random, encapsulated with its MAC address in the data message. Data messages are sent in quantum information, i.e. using density operators. The protocol determines whether the newly selected IP address is already in use by broadcasting a probe loading the message. If a host responds to the probe, which means that the IP address is occupied, the protocol updates the message with a new IP address. If no host responds within a unit of time, which may be caused by missing probes. Finally, a server on the LAN records the new host’s IP and MAC addresses in the message after transferring through the noisy channel. Hence the fidelity between the initial MAC address and the final one is worth evaluating for the reliability of the channel.

The QMC \( \mathcal{C} = (S, Q, L) \) in Figure [1] describes the quantum IPv4 protocol. The state set \( S \) is \( \{s_0, s_1, s_2, s_3, s_4, s_5\} \), where \( L(s_2) = \{\text{ok}\} \), \( L(s_4) = \{\text{error}\} \), and other states are labelled with \( \emptyset \). The state \( s_0 \) indicates that a new host joins in a LAN. The states \( s_i \ (i = 1, 2, 3, 4) \) indicate although the address is occupied, no host responds the probe within \( i \) units of time. If the total time \( i = 4 \) does not run out, re-broadcasting a probe would take place, which leads to returning to the state \( s_0 \); otherwise the state \( s_5 \) indicates a wrong IP address configuration. The state \( s_3 \) indicates a proper IP address configuration. The transition super-operator matrix \( Q \) is given by the following nonzero entries in Kraus representation [1]:

\[
\begin{align*}
Q(s_0, s_1) &= \frac{1}{\sqrt{2}} |+\rangle \langle 1|, & Q(s_0, s_3) &= \frac{1}{\sqrt{2}} |2\rangle \langle 1|, \\
Q(s_1, s_0) &= \frac{1}{\sqrt{2}} |+\rangle \langle 1|, & Q(s_1, s_3) &= \frac{1}{\sqrt{2}} |2\rangle \langle 1|, \\
Q(s_0, s_2) &= \frac{1}{\sqrt{2}} |X\rangle \langle I|, & Q(s_2, s_1) &= \frac{1}{\sqrt{2}} |I\rangle \langle X|, \\
Q(s_3, s_0) &= \frac{1}{\sqrt{2}} |Z\rangle \langle I|, & Q(s_3, s_4) &= \frac{1}{\sqrt{2}} |I\rangle \langle Z|, \\
Q(s_4, s_1) &= |I\rangle \langle I|.
\end{align*}
\]

where \( |\pm\rangle = (|1\rangle \pm |2\rangle) / \sqrt{2} \), \( I = |1\rangle \langle 1| + |2\rangle \langle 2| \) is the identity operator, \( X = |1\rangle \langle 2| + |2\rangle \langle 1| \) is the bit flip and \( Z = |1\rangle \langle 1| - |2\rangle \langle 2| \) is the phase flip. It is easy to validate that \( \sum_{s \in S} Q(s, i) \approx I \) holds for each \( s \in S \).

We can combine all these super-operators on \( \mathcal{H} \) as a single super-operator on \( \mathcal{H}_{\text{q}} \):

\[
\mathcal{F} = \{|s_1\rangle\langle s_0| \otimes Q(s_0, s_1) + |s_3\rangle\langle s_2| \otimes Q(s_2, s_3) + |s_0\rangle\langle s_1| \otimes Q(s_1, s_0) +
|s_2\rangle\langle s_1| \otimes Q(s_1, s_2) + |s_0\rangle\langle s_2| \otimes Q(s_2, s_0) + |s_3\rangle\langle s_2| \otimes Q(s_2, s_3) +
|s_0\rangle\langle s_3| \otimes Q(s_3, s_0) + |s_4\rangle\langle s_3| \otimes Q(s_3, s_4) + |s_4\rangle\langle s_4| \otimes I + |s_5\rangle\langle s_5| \otimes I,\]
\]

These super-operator entries are modelling noisy channels. In practice, each of them has a large proportion of being the identity operator \( I \) with a small proportion of being noise operators, e.g. the bit flip \( X \) and the phase flip \( Z \), which would change density operators. However, to present our method concisely, we focus more on the situation where severe noises appear. Thus we set super-operator entries simply by those noise operators.
in which the left operand of the tensor product in a term is a super-operator on $C$ and the right operand is a super-operator on $\mathcal{H}$.

Figure 1: QMC for IPv4 protocol

In the QMC $\mathcal{C}_1$, $\omega_1 = s_3 s_0 s_1 s_0 s_3 s_5 s_\cdots$ is a path starting in $s_3$, where $\omega_1(0) = s_3$, $\omega_1(1) = \omega_1(3) = s_0$, $\omega_1(2) = s_1$, and $\omega_1(i) = s_5$ for $i \geq 4$; while $\hat{\omega}_1 = s_3 s_0 s_1 s_0 s_3$ is a finite prefix of $\omega_1$. Therefore, we have $\omega_1 \in \text{Path}(s_3)$ and $\hat{\omega}_1 \in \text{Path}_{\text{fin}}(s_3)$.

To reason about quantitative properties of QMC, a super-operator valued measure (SOVM) space over paths could be established as follows. Recall that:

**Definition 3.3.** A measurable space is a pair $(\Omega, \Sigma)$, where $\Omega$ is a nonempty set and $\Sigma$ is a $\sigma$-algebra on $\Omega$; in addition an SOVM space is a triple $(\Omega, \Sigma, \Delta)$, where $(\Omega, \Sigma)$ is a measurable space and $\Delta : \Sigma \rightarrow S^\leq I$ is an SOVM, satisfying:

- $\Delta(\Omega) \approx I$, and
- $\Delta(\bigcup_i A_i) \equiv \sum_i \Delta(A_i)$ for any pairwise disjoint $A_i \in \Sigma$.

For a given finite path $\hat{\omega} \in \text{Path}_{\text{fin}}(s)$, we define the cylinder set as

$$\text{Cyl}(\hat{\omega}) := \{ \omega \in \text{Path}(s) : \omega \text{ has the prefix } \hat{\omega} \};$$

and for $B \subseteq \text{Path}_{\text{fin}}(s)$, we extend (4) by $\text{Cyl}(B) := \bigcup_{\hat{\omega} \in B} \text{Cyl}(\hat{\omega})$. Particularly, we have $\text{Cyl}(s) = \text{Path}(s)$. Let $\Omega = \text{Path}(s)$ for an appointed $s \in S$, and $\Pi \subseteq 2^\Omega$ be the countable set of all cylinder sets $\{\text{Cyl}(\hat{\omega}) : \hat{\omega} \in \text{Path}_{\text{fin}}(s)\}$ plus the emptyset $\emptyset$. By [4, Chapt. 10], there is a smallest $\sigma$-algebra $\Sigma$ of $\Pi$ that contains $\Pi$ and is closed under countable union and complement. It is clear that the pair $(\Omega, \Sigma)$ forms a measurable space.

Next, for a given finite path $\hat{\omega} = s_0 s_1 \cdots s_n$, we define the accumulated super-operator along with $\hat{\omega}$ as

$$\Delta(\text{Cyl}(\hat{\omega})) := \begin{cases} I & \text{if } n = 0, \\ Q(s_{n-1}, s_n) \circ \cdots \circ Q(s_0, s_1) & \text{otherwise}. \end{cases}$$

By [12, Thm. 3.2], the domain of $\Delta$ can be extended to $\Sigma$, i.e. $\Delta : \Sigma \rightarrow S^\leq I$, which is unique under the countable union $\bigcup_i A_i$ for any $A_i \in \Pi$ and is an equivalence class of super-operators in terms of $\approx$ under the complement $A^C$ for some $A \in \Pi$. Hence the triple $(\Omega, \Sigma, \Delta)$ forms an SOVM space.
4. Quantum Computation Tree Logic

We now introduce a quantum extension of computation tree logic (QCTL). The basic idea is to replace the probability measure in the logic of \[13\] with fidelity. As we mentioned in the introduction, fidelity is useful in comparing quantum states. In practice, the preparation of any quantum state is limited by imperfections and noises, and one often needs to find out how close the produced state is to the intended one. In many occasions, fidelity can detect the effect of a noisy channel but probability measure cannot.

In the following, we present the syntax and semantics of the new logic, then compare it with probabilistic CTL (PCTL) [20] and with the QCTL presented in [12].

**Definition 4.1.** The syntax of QCTL consists of the state formulas $\Phi$ and path formulas $\phi$:

$$
\Phi := a | \neg \Phi | \Phi_1 \land \Phi_2 | Cyl(\tau)[\phi]
$$

$$
\phi := X \Phi | \Phi_1 \cup \Phi_2 | \Phi_1 \cup \Phi_2
$$

where $a \in AP$ is an atomic proposition, $\sim \in \{<, \leq, =, \geq, >\}$ is a comparison operator, $\tau \in Q \cap [0, 1]$ is a threshold, and $k \geq 0$ is a step bound.

The state formula $Cyl(\tau)[\phi]$ in QCTL is called the fidelity-quantifier formula, and other state formulas are basic ones. The three kinds of path formulas $X \Phi, \Phi_1 \cup \Phi_2$ and $\Phi_1 \cup \Phi_2$ are the next, the bounded-until and the unbounded-until formulas, respectively.

**Definition 4.2.** The semantics of QCTL interpreted over a QMC $\mathcal{E} = (S, Q, L)$ is given by the satisfaction relation $\models$:

- $s \models a$ if $a \in L(s)$,
- $s \not\models \neg \Phi$ if $s \not\models \Phi$,
- $s \models \Phi_1 \land \Phi_2$ if $s \models \Phi_1$ and $s \models \Phi_2$,
- $s \models Cyl(\tau)[\phi]$ if $\text{Fid}(\Delta(\omega \in \text{Path}(s) : \omega \models \phi)) \sim \tau$,
- $\omega \models X \Phi$ if $\omega(1) \models \Phi$,
- $\omega \models \Phi_1 \cup \Phi_2$ if $\exists i \leq k : (\omega(i) \models \Phi_2 \land \forall j < i : \omega(j) \models \Phi_1)$,
- $\omega \models \Phi_1 \cup \Phi_2$ if $\exists i : (\omega(i) \models \Phi_2 \land \forall j < i : \omega(j) \models \Phi_1)$.

Other logic connectives $\lor, \rightarrow$ and $\leftrightarrow$ can be easily derived by $\neg$ and $\land$ as usual.

For any path formula $\phi$, the path set $A = \{\omega \in \text{Path}(s) : \omega \models \phi\}$ is measurable, since

- if $\phi = X \Phi$, $A$ is the finite union of those cylinder sets $\text{Cyl}(st)$ that satisfy $t \models \Phi$;
- if $\phi = \Phi_1 \cup \Phi_2$, $A$ is the finite union of $\text{Cyl}(s_0 \cdots s_i)$ for some $i \leq k$, that satisfy $s_0 = s$, $s_i \models \Phi_2$, and $s_j \models \Phi_1$ for each $j < i$; and
- if $\phi = \Phi_1 \cup \Phi_2$, $A$ is the countable union of $\text{Cyl}(s_0 \cdots s_i)$ for some $i \geq 0$, that satisfy $s_0 = s$, $s_i \models \Phi_2$, and $s_j \models \Phi_1$ for each $j < i$.

Thereby, the set $A$ belongs to the $\sigma$-algebra $\Sigma$ and in particular is a countable union of cylinder sets, which entails that the SOVM $\Delta(A)$ is uniquely defined. For conciseness, we will write $\Delta(\hat{\omega})$ for $\Delta(\text{Cyl}(\hat{\omega}))$ and $\Delta(\phi)$ for $\Delta(\{\omega \in \text{Path}(s) : \omega \models \phi\})$ afterwards.
Example 4.3. From the QMC $\mathcal{E}_1$ together with the path $\omega_1 = s_3 s_0 s_1 s_0 s_3 s_5 \cdots$ shown in Example \[\text{2.6}\] we can see

- $s_5 \models \text{ok}$ and $s \not\models \text{ok}$ for each $s \in S \setminus \{s_5\}$;
- $\omega_1 \models \text{true} \cup \text{ok}$, as $\omega_1(4) \models \text{ok}$ and $\omega_1(j) \models \text{true}$ for each $j < 4$.

For each $s \in S$, we can establish an SOVM space $(\Omega, \Sigma, \Delta)$ over the path set $\text{Path}(s)$ of $\mathcal{E}_1$. To demonstrate the generality of the method developed in this paper, we choose $\Omega = \text{Path}(s_3)$. The SOVM $\Delta(\omega_1)$ is calculated as

$$\Delta(\omega_1) = \Delta(\text{Cyl}(\omega_1)) = Q(s_0, s_5) \circ Q(s_1, s_0) \circ Q(s_0, s_1) \circ Q(s_3, s_0)$$

where the last equation follows from the fact that they are two Kraus representations of a super-operator $\phi$ with the threshold $\tau$, and decides it over a QMC with a specific initial state (density operator).

In details, we calculate the composition of super-operators using right associativity law, e.g.

$$Q(s_0, s_1) \circ Q(s_3, s_0)$$

where the last equation follows from the fact that they are two Kraus representations of a super-operator. Since $\omega_1 \in \Omega$ and $\omega_1 \models \text{true} \cup \text{ok}$, we have the lower bound $\Delta(\text{true} \cup \text{ok}) \geq \{\frac{576\sqrt{48}}{3125}|1, 2\}(1, 2)$.

Finally, we point out the difference between the PCTL in \[\text{2.6}\], the QCTL in \[\text{1.2}\] and our QCTL. The PCTL extends CTL by introducing a probability-quantifier $\exists_{\leq \tau}(\phi)$ that compares the probability of the measurable event specified by $\phi$ with the threshold $\tau$, and decides it over a MC with a specific initial state (probability distribution). The QCTL in \[\text{1.2}\] introduces an SOVM-quantifier $\exists_{\leq \tau}(\phi)$ that compares the SOVM on $\phi$ with the super-operator threshold $E$ under the trace pre-order $\lesssim$; and decides it over a QMC with a specific initial state (density operator). Whereas, ours introduces a fidelity-quantifier $\exists_{\leq \tau}(\phi)$ that compares the fidelity of the SOVM on $\phi$ with the threshold $\tau$; and aims to decide it over a QMC with a parametric initial state. The parametric model is more expressive, and thus our method would be potentially more applicable. How to consider the SOVM-quantifier on a parametric QMC would be one of our future work.
5. Model Checking Algorithm

In this section, we present the model checking algorithm for a given QMC $\mathcal{C} = (S, Q, L)$ and a QCTL state formula $\Phi$. The algorithm would decide $s \models \Phi$ for an appointed state $s \in S$, or equivalently compute the set of all states satisfying $\Phi$, i.e. $\text{Sat}(\Phi) := \{ s \in S : s \models \Phi \}$. Since the definition of QCTL is mutually inductive, this goal will be reached in three steps:

1. deciding basic state formulas (except for the fidelity-quantifier one),
2. synthesizing the super-operators of path formulas, and
3. deciding the fidelity-quantifier formula.

5.1. Deciding basic state formulas

For basic state formulas, the satisfying sets are calculated by their definitions:

- $\text{Sat}(a) = \{ s \in S : a \in L(s) \}$;
- $\text{Sat}(\neg \Phi) = S \setminus \text{Sat}(\Phi)$, provided that $\text{Sat}(\Phi)$ is known; and
- $\text{Sat}(\Phi_1 \land \Phi_2) = \text{Sat}(\Phi_1) \cap \text{Sat}(\Phi_2)$, provided that $\text{Sat}(\Phi_1)$ and $\text{Sat}(\Phi_2)$ are known.

Obviously, the top-level logic connective of those formulas requires merely a scan over the labelling function $L$ on $S$, which is in $O(n)$. Hence, deciding basic state formulas is linear time w.r.t. the size of $\mathcal{C}$.

Example 5.1. From the QMC $\mathcal{C}_1$ shown in Example 3.2 it is easy to calculate

- $\text{Sat}(\text{ok}) = \{ s_3 \}$, $\text{Sat}(\text{error}) = \{ s_4 \}$;
- $\text{Sat}(\neg \text{ok}) = S \setminus \text{Sat}(\text{ok}) = \{ s_0, s_1, s_2, s_3, s_4 \}$;
- $\text{Sat}(\neg \text{error}) = S \setminus \text{Sat}(\text{error}) = \{ s_0, s_1, s_2, s_3, s_4 \}$; and
- $\text{Sat}(\text{ok} \lor \text{error}) = \text{Sat}(\neg \text{ok} \land \neg \text{error}) = \text{Sat}(\neg \text{ok}) \cap \text{Sat}(\neg \text{error}) = \{ s_0, s_1, s_2, s_3 \}$.

5.2. Synthesizing the super-operators of path formulas

Let $P_s$ denote the projection super-operator $|s\rangle\langle s| \otimes I = |s\rangle\langle s| \otimes I$ on the enlarged Hilbert space $\mathcal{H}_s$, and $P_\Phi := \sum_{s \in S} |s\rangle\langle s| \otimes I = |\sum_{s \in S} |s\rangle\langle s| \otimes I|$. Utilizing the mixed structure of the classical–quantum state $\rho = \sum_{s \in S} |s\rangle\langle s| \otimes \rho_s$, we have the nice property

$$\rho = \sum_{s \in \Phi} |s\rangle\langle s| \otimes \rho_s + \sum_{s \notin \Phi} |s\rangle\langle s| \otimes \rho_s = P_\Phi(\rho) + P_{\neg \Phi}(\rho)$$  \hspace{1cm} (6)

So, fixing an initial classical state $s$, we can obtain the SOVMs of path formulas as follows.

- Supposing that $\text{Sat}(\Phi)$ is known, we have

$$\Delta(X \Phi) = \sum_{s \in \Phi} Cyl(s, t) = \sum_{s \in \Phi} \Delta(s, t) = \sum_{s \notin \Phi} Q(s, t),$$  \hspace{1cm} (7a)

where $\cup$ denotes disjoint union.
Supposing that \( \text{Sat}(\Phi_1) \) and \( \text{Sat}(\Phi_2) \) are known, we have
\[
\Delta(\Phi_1 \cup \Phi_2) = \Delta \left( \bigcup_{i=0}^{k} \left\{ \omega \in \text{Path}(s) : \omega(i) \models \Phi_2 \land \bigwedge_{j=0}^{i-1} \omega(j) \models \Phi_1 \land \neg \Phi_2 \right\} \right)
\]
\[
= \sum_{i=0}^{k} \Delta \left( \left\{ \omega \in \text{Path}(s) : \omega(i) \models \Phi_2 \land \bigwedge_{j=0}^{i-1} \omega(j) \models \Phi_1 \land \neg \Phi_2 \right\} \right)
\]
\[
= \sum_{i=0}^{k} \text{tr}_C(P_{\Phi_2} \circ (F \circ P_{\Phi_1 \lor \neg \Phi_2})^i \circ P_s),
\]
where \( \text{tr}_C = \{|s| \otimes I : s \in S\} \) is the partial trace that traces out the classical system \( C \) and \( F = \sum_{s \in S} |l(s)||l(s) \otimes Q(s, t) \) is defined in Section 3.

Supposing that \( \text{Sat}(\Phi_1) \) and \( \text{Sat}(\Phi_2) \) are known, we have
\[
\Delta(\Phi_1 \cup \Phi_2) = \Delta \left( \bigcup_{i=0}^{\infty} \left\{ \omega \in \text{Path}(s) : \omega(i) \models \Phi_2 \land \bigwedge_{j=0}^{i-1} \omega(j) \models \Phi_1 \land \neg \Phi_2 \right\} \right)
\]
\[
= \sum_{i=0}^{\infty} \Delta \left( \left\{ \omega \in \text{Path}(s) : \omega(i) \models \Phi_2 \land \bigwedge_{j=0}^{i-1} \omega(j) \models \Phi_1 \land \neg \Phi_2 \right\} \right)
\]
\[
= \sum_{i=0}^{\infty} \text{tr}_C(P_{\Phi_2} \circ (F \circ P_{\Phi_1 \lor \neg \Phi_2})^i \circ P_s).
\]

For the latter two cases, we classify all satisfying paths \( \omega \) upon the first timestamp \( i \) that satisfies \( \omega(i) \models \Phi_2 \) and \( \omega(j) \models \Phi_1 \) for each \( j < i \) (or equivalently the unique timestamp \( i \) that satisfies \( \omega(i) \models \Phi_2 \) and \( \omega(j) \models \Phi_1 \lor \neg \Phi_2 \) for each \( j < i \)). Thereby, the resulting sets \( A_i = \{ \omega \in \text{Path}(s) : \omega(i) \models \Phi_2 \land \bigwedge_{j=0}^{i-1} \omega(j) \models \Phi_1 \land \neg \Phi_2 \} \) are pairwise disjoint, and their SOVMs are obtained as \( \text{tr}_C(P_{\Phi_2} \circ (F \circ P_{\Phi_1 \lor \neg \Phi_2})^i \circ P_s) \).

We notice that all super-operators, say \( F \circ P_{\Phi_1 \lor \neg \Phi_2} \), in the SOVMs \( \{ \} \) has the property \( F \circ P_{\Phi_1 \lor \neg \Phi_2} = F \circ P_{\Phi_1 \lor \neg \Phi_2} \circ \sum_{s \in S} P_s \), which implies all density operators \( \rho \in \mathcal{D}(\mathcal{H}_i) \) occurring in our analysis keep the mixed structure \( \sum_{s \in S} \langle s| \otimes \rho_s \) with \( \rho_s \in \mathcal{D} \).

**Example 5.2.** Under the SOVM space \( (\Omega, \Sigma, \Delta) \) established in Example 4.3 we consider the path formula \( \phi_1 = \text{true} \cup \text{ok} \). The satisfying path sets are disjoint \( A_i = \{ \omega \in \Omega : \omega(i) \models \text{ok} \land \bigwedge_{j=0}^{i-1} \omega(j) \models \neg \text{ok} \} \) \( (i \geq 0) \); and their SOVMs are:
\[
\Delta(A_0) = \text{tr}_C(P_{\text{ok}} \circ P_{s_1}) = 0,
\]
\[
\Delta(A_1) = \text{tr}_C(P_{\text{ok}} \circ (F \circ P_{\neg\text{ok}}) \circ P_{s_1}) = 0,
\]
\[
\Delta(A_2) = \text{tr}_C(P_{\text{ok}} \circ (F \circ P_{\neg\text{ok}})^2 \circ P_{s_1}) = \frac{125}{125} \left| 1, 2 \right>(1, 2) \left| 1, 2 \right> \otimes Z, 
\]
\[
\Delta(A_3) = \text{tr}_C(P_{\text{ok}} \circ (F \circ P_{\neg\text{ok}})^3 \circ P_{s_1}) = 0,
\]
\[
\Delta(A_4) = \text{tr}_C(P_{\text{ok}} \circ (F \circ P_{\neg\text{ok}})^4 \circ P_{s_1}) = \frac{576}{125} \left| 1, 2 \right>(1, 2),
\]
\[
\Delta(A_5) = \text{tr}_C(P_{\text{ok}} \circ (F \circ P_{\neg\text{ok}})^5 \circ P_{s_1}) = \frac{1272}{15025} \left| 2, 2 \right>(1, 2).
\]

and so on.
Although the three kinds of path formulas have the SOVMs (\((7)\), the super-operators are not expressed in an explicit form, i.e. there are too many Krusz operators to make up the super-operators \(\Delta(\phi)\). In particular, \(\Delta(\Phi_1 \cup \Phi_2)\) in \((7)\) is even not expressed in a closed form. In the following, we will construct explicit matrix representations for these super-operators, particularly for \(\Delta(\Phi_1 \cup \Phi_2)\). A natural idea is:

1. using the matrix representation of \(\Delta(\Phi_1 \cup \Phi_2)\), which is analogous to a geometric series with common ratio—the matrix representation of \(\mathcal{F}_{\Phi_1 \cup \Phi_2} : = \mathcal{F} \circ \mathcal{F}_{\Phi_1 \cup \Phi_2}\); and
2. reformulating it as a matrix fraction.

However, \(\mathcal{F}_{\Phi_1 \cup \Phi_2}\) may have some fixed-point \(\gamma\) (or equivalently the matrix representation of \(\mathcal{F}_{\Phi_1 \cup \Phi_2}\) may have eigenvalue 1), which makes the matrix fraction divergent. To overcome the trouble, inspired by \((1)\), we will remove the bottom strongly connected component (BSCC) subspaces \(\Gamma\) that cover all fixed-points \(\gamma \in \mathcal{F}_{\Phi_1 \cup \Phi_2}\), i.e. \(\text{supp}(\gamma) \subseteq \Gamma\). Recall that:

**Definition 5.3.** For a super-operator \(\mathcal{E} \in \mathcal{S}\), a subspace \(\Gamma \in \mathcal{H}\) is bottom if for any pure state \(|\psi\rangle \in \Gamma\), the support of \(\mathcal{E}(|\psi\rangle\langle\psi|)\) is contained in \(\Gamma\); it is SCC if for any pure states \(|\psi_1\rangle, |\psi_2\rangle \in \Gamma\), \(|\psi_1\rangle \langle\psi_2|\) is in \(\text{span}(\bigcup_{i=0}^{\infty} \text{supp}(\mathcal{E}(\langle\psi_i|\langle\psi_i|)))); and it is BSCC if it is bottom and SCC.

We characterize the fixed-point of \(\mathcal{F}_{\Phi_1 \cup \Phi_2}\) by the stationary equation

\[
\mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma) = \gamma \quad (\gamma = \gamma \in \mathcal{L}(\mathcal{H}_m)),
\]

where \(\gamma\) are unknown variables and \(\mathcal{F}_{\Phi_1 \cup \Phi_2}\) gives rise to coefficients. It is a system of homogeneous linear equations. Let \(\gamma_j (i \in [m])\) be all linearly independent solutions of \((8)\). Thanks to the property \(\mathcal{F}_{\Phi_1 \cup \Phi_2} = \mathcal{F}_{\Phi_1 \cup \Phi_2} \circ \sum_{E \in \mathcal{S}} \mathcal{P}_E\), the number of real variables in the Hermitian operator \(\gamma\) can be bounded by \(nm^2\). So the number \(m\) of these solutions is also bounded by \(nm^2\). We proceed to find out the BSCC subspaces by the following lemma.

**Lemma 5.4.** The direct-sum of all BSCC subspaces w.r.t. \(\mathcal{F}_{\Phi_1 \cup \Phi_2}\) is \(\text{span}(\bigcup_{i=0}^{m} \text{supp}(\gamma_j))\).

**Proof.** We first prove \(\Gamma := \text{span}(\bigcup_{i=0}^{m} \text{supp}(\gamma_j))\) is the direct-sum of some BSCC subspaces that covers all fixed-point of \(\mathcal{F}_{\Phi_1 \cup \Phi_2}\); then show it is the direct-sum of all BSCC subspaces.

Let \(\gamma_j = \sum_{i=0}^{n} \lambda_{i,j} |\psi_{i,j}\rangle\langle\psi_{i,j}|\) be the spectral decomposition of \(\gamma_j\), where \(\lambda_{i,j} \in \mathbb{R} (j \in [N])\) are all eigenvalues of \(\gamma_j\) and \(|\psi_{i,j}\rangle\) are the corresponding eigenvectors. Define

\[
\gamma_j^+ := \sum_{\lambda_{i,j} \lambda_{i,j} > 0} ||\lambda_{i,j} |\psi_{i,j}\rangle\langle\psi_{i,j}| : j \in [N] \wedge \lambda_{i,j} > 0 ||
\]

and

\[
\gamma_j^- := \sum_{\lambda_{i,j} \lambda_{i,j} < 0} ||\lambda_{i,j} |\psi_{i,j}\rangle\langle\psi_{i,j}| : j \in [N] \wedge \lambda_{i,j} < 0 ||,
\]

where \(|| \cdot ||\) denotes a multiset, as the positive and the negative parts of \(\gamma_j\), respectively. Utilizing the fact that \(\mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma_j)\) is exactly \(\mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma_j^+)\) while the negative part of \(\mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma_j)\) is \(\mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma_j^-)\). Since \(\mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma_j) = \gamma_j\), we have \(\mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma_j^+) = \gamma_j^+\) and \(\mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma_j^-) = \gamma_j^-\). So we can see that \(\gamma_j^+\) and \(-\gamma_j^-\) are positive solutions of \((8)\) that together can linearly express any solution of \((8)\).

Fixed a positive solution \(\gamma = \sum \lambda_{i,j} |\psi_{i,j}\rangle\langle\psi_{i,j}|\) in the solution set \(\{\gamma_i^+ : i \in [m]\} \cup \{-\gamma_i^- : i \in [m]\} \setminus \{0\}\), we have

\[
\gamma - \lambda_{i,j} \mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma_{i,j}) = \mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma) - \lambda_{i,j} \mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma_{i,j})
\]

and

\[
= \mathcal{F}_{\Phi_1 \cup \Phi_2}(\gamma - \lambda_{i,j} |\psi_{i,j}\rangle\langle\psi_{i,j}|)
\]

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is positive for each \( |\Psi_j \rangle \) \((j \in [m])\), which implies \( \text{supp}(F_{\Phi_1 \wedge \Phi_2}(|\Psi_j \rangle \langle \Psi_j |)) \) is contained in \( \text{supp}(\gamma) \). In other words, for any Kraus operator \( F_\ell \) of \( F_{\Phi_1 \wedge \Phi_2}, F_\ell |\Psi_j \rangle \) is in \( \text{supp}(\gamma) \), i.e. \( \sum_j |\Psi_j \rangle \langle \Psi_j | F_\ell = F_\ell |\Psi_j \rangle \). Furthermore, for any \( |\Psi \rangle \in \text{supp}(\gamma) \), after expressing it as \( \sum_j c_j |\Psi_j \rangle \) with \( \sum_{i \in [d]} |c_i|^2 = 1 \), we have

\[
\begin{align*}
\left( \sum_j |\Psi_j \rangle \langle \Psi_j | \right) F_{\Phi_1 \wedge \Phi_2}(|\Psi \rangle \langle \Psi |) \\
= \left( \sum_j |\Psi_j \rangle \langle \Psi_j | \right) \left( \sum_{\ell} F_\ell \left( \sum_j \sum_i c_i |\Psi_j \rangle \langle \Psi_i | \right) F_\ell^\dagger \right) \\
= \sum_{\ell} F_\ell \left( \sum_j \sum_i c_i |\Psi_j \rangle \langle \Psi_i | \right) F_\ell^\dagger \\
= F_{\Phi_1 \wedge \Phi_2}(|\Psi \rangle \langle \Psi |),
\end{align*}
\]

which implies \( \text{supp}(F_{\Phi_1 \wedge \Phi_2}(|\Psi \rangle \langle \Psi |)) \) is contained in \( \text{supp}(\gamma) \). Thus \( \text{supp}(\gamma) \) is bottom w.r.t. \( F_{\Phi_1 \wedge \Phi_2} \). Additionally, \( \text{span}(\bigcup_{i \in [m]} \text{supp}(F_i^0(|\Psi_j \rangle \langle \Psi_j |))) \) forms a BSCC subspace w.r.t. \( F_{\Phi_1 \wedge \Phi_2} \). Hence, \( \text{supp}(\gamma) \) is the direct-sum of some BSCC subspaces of \( \mathcal{H}_{\text{eq}} \) as well as \( \Gamma \). The latter covers all fixed-points of \( F_{\Phi_1 \wedge \Phi_2} \), since any fixed-point of \( F_{\Phi_1 \wedge \Phi_2} \) can be linearly expressed by \( \{ \gamma_i^* : i \in [m] \} \cup \{-\gamma_i^*: i \in [m]\} \), whose supports are contained in \( \Gamma \).

We proceed to prove that \( \Gamma \) is the direct-sum of all BSCC subspaces. By the decomposition \([31] \text{Thm. 5} \) and \([17] \text{Thm. 1} \), we have

\[
\mathcal{H}_{\text{eq}} = \mathcal{T} \oplus \bigoplus_i \Gamma_i,
\]

where \( \mathcal{T} \) is the maximal transient subspace w.r.t. \( F_{\Phi_1 \wedge \Phi_2} \) and each \( \Gamma_i \) is a BSCC subspace; and although the decomposition is not unique, the maximal transient subspace \( \mathcal{T} \) is unique as well as the direct-sum of all BSCC subspaces \( \Gamma_i \). We assume by contradiction that \( \Gamma \) does not contain all BSCC subspaces. Then there is a BSCC subspace \( \Gamma_0 \) orthogonal to \( \Gamma \). It is easy to see that

- the set \( D_{\text{eq}}^1 \) of density operators \( \rho \) on \( \Gamma_0 \) with trace 1 is a convex and compact set in the viewpoint of probabilistic ensemble form \( \{(p_i, |\psi_i \rangle) : i \in [d]\} \) that is obtained from the spectral decomposition \( \rho = \sum_{i \in [d]} p_i |\psi_i \rangle \langle \psi_i | \); and
- \( F_{\Phi_1 \wedge \Phi_2} \) is a continuous function mapping \( D_{\text{eq}}^1 \) to itself.

By Brouwer’s fixed-point theorem \([22] \text{Chap. 4} \) that for a continuous function \( f \) mapping a convex and compact set \( \chi \) to itself, there is a point \( x \in \chi \) such that \( f(x) = x \), we know there is a fixed-point \( \rho_0 \) of \( F_{\Phi_1 \wedge \Phi_2} \) in \( D_{\text{eq}}^1 \). From the construction of \( \Gamma \), however, we have \( \text{supp}(\rho_0) \subseteq \Gamma \), which implies \( \Gamma_0 \) is not orthogonal to \( \Gamma \) and thus contradicts the assumption. Hence we obtain that \( \Gamma \) is exactly the direct-sum of all BSCC subspaces w.r.t. \( F_{\Phi_1 \wedge \Phi_2} \). \( \square \)

We formally describe the procedure to compute the direct-sum \( \Gamma \) of all BSCC subspaces w.r.t. \( F_{\Phi_1 \wedge \Phi_2} \) as Algorithm\([1] \). By invoking it on the super-operator \( F_{\Phi_1 \wedge \Phi_2} \) and the Hilbert space \( \mathcal{H}_{\text{eq}} \),
we would obtain the direct-sum \( \Gamma \) in \( O(N^6) \) arithmetic operations, which is more efficient than the existing method \(^1\) Procedure GetBSCC in \( O(N^7) \) field operations.\(^2\)

Algorithm 1 Computing the direct-sum of all BSCC subspaces.

\[
\Gamma \leftarrow \text{BSCC}(E, H)
\]

**Input:** \( E \in S \) is a super-operator on the Hilbert space \( \mathcal{H} \) of dimension \( d \).

**Output:** \( \Gamma \) is the direct-sum of all BSCC subspaces w.r.t. \( E \).

1: \( \Gamma \leftarrow \{0\}; \quad \triangleright \text{initializing } \Gamma \text{ as the zero space}
2: \text{compute all linearly independent solutions } \gamma_i \text{ (} i \in [m] \text{) of } \mathcal{E}(\gamma) = \gamma (\gamma = \gamma^\dagger \in \mathcal{L}_H);
3: \text{for each } i \in [m] \text{ do}
4: \quad \Gamma \leftarrow \text{span}(\Gamma \cup \text{supp}(\gamma_i));
5: \text{return } \Gamma .

**Complexity.** In Algorithm\(^1\) the stationary equation \( \gamma = \mathcal{E}(\gamma) \) can be solved in \( O(d^6) \) by Gaussian elimination, whose complexity is cubic in the number \( d^2 \) of real variables in \( \gamma \). The support \( \text{supp}(\gamma_i) \) of an individual solution \( \gamma_i \) and the extended space \( \text{span}(\Gamma \cup \text{supp}(\gamma_i)) \) can be computed in \( O(d^3) \) by the Gram–Schmidt procedure, whose complexity is cubic in the dimension \( d \). In total, they are in \( O(md^3) \subseteq O(d^7) \), as the number \( m \) of linearly independent solutions is bounded by \( d^2 \).

Let \( \mathcal{P}_T = \{P_t\} \) where \( P_t \) is the projector onto \( \Gamma_t \), i.e. \( \mathcal{P}_T(H_{eq}) = \Gamma_t \); and \( \mathcal{P}_{T^\perp} = \{P_{t^\perp}\} \) where \( \Gamma_t^\perp \) is the orthogonal complement of \( \Gamma_t \), i.e. \( \Gamma_t \otimes \Gamma_t^\perp = H_{eq} \). Again, thanks to the fact the states in the QMC are of the mixed structure \( \rho = \sum_{s \in S} |s\rangle \langle s| \otimes P_s \), we have that \( \mathcal{P}_T \) is of the form \( \sum_{s \in S} |s\rangle \langle s| \otimes P_s \) where \( P_s \) (\( s \in S \)) are positive operators, as well as \( \mathcal{P}_{T^\perp} = I_{H_{eq}} - \mathcal{P}_T \).

**Example 5.5.** Consider the path formula \( \phi_4 = \text{true} \cup \langle \omega \leq 15 \rangle \langle \omega \vee \text{error} \rangle \) on the QMC \( \Xi_1 \) in Example 5.2. The repeated super-operator in the SOVM \( \Delta(\phi_4) \) is

\[
\mathcal{F}^\omega - \text{error} := \mathcal{F} \circ \mathcal{P}^\omega - \text{error} = \mathcal{F} \circ \mathcal{P}^\text{true} \setminus (\omega \vee \text{error})
\]

\[
= \begin{cases}
|s\rangle |s_0\rangle \otimes [1, +] |1, 1, \frac{1}{4} |s_1\rangle |s_0\rangle \otimes [1, -] |1, 2, \frac{1}{4} |s_2\rangle |s_0\rangle \otimes [1, 1, +] |1, 2, \frac{1}{4} |s_3\rangle |s_0\rangle \otimes [1, 2, +] |1, 1, \frac{1}{4} |s_4\rangle |s_0\rangle \otimes [1, -] |1, 2, \frac{1}{4} |s_5\rangle |s_0\rangle \otimes [1, 2, +] |1, 1, \frac{1}{4} |s_6\rangle |s_0\rangle \otimes [1, -] |1, 2, \frac{1}{4} |s_7\rangle |s_0\rangle \otimes [1, 2, +] |1, 1, \frac{1}{4} |s_8\rangle |s_0\rangle \otimes [1, -] |1, 2, \frac{1}{4} |s_9\rangle |s_0\rangle \otimes [1, 2, +] |1, 1, \frac{1}{4} |s_{10}\rangle |s_0\rangle \otimes [1, -] |1, 2, \frac{1}{4} |s_{11}\rangle |s_0\rangle \otimes [1, 2, +] |1, 1, \frac{1}{4} |s_{12}\rangle |s_0\rangle \otimes [1, -] |1, 2, \frac{1}{4} |s_{13}\rangle |s_0\rangle \otimes [1, 2, +] |1, 1, \frac{1}{4} |s_{14}\rangle |s_0\rangle \otimes [1, -] |1, 2, \frac{1}{4} |s_{15}\rangle |s_0\rangle \otimes [1, 2, +] |1, 1, \frac{1}{4} |s_{16}\rangle |s_0\rangle \otimes [1, -] |1, 2, \frac{1}{4} |s_{17}\rangle |s_0\rangle \otimes [1, 2, +] |1, 1, \frac{1}{4} |s_{18}\rangle |s_0\rangle \otimes [1, -] |1, 2, \frac{1}{4} |s_{19}\rangle |s_0\rangle \otimes [1, 2, +] |1, 1, \frac{1}{4} \end{cases}.
\]

Solving the stationary equation \( \mathcal{F}^\omega - \text{error} \gamma = \gamma (\gamma = \gamma^\dagger \in \mathcal{L}_H) \), we obtain only one solution \( \gamma_1 = |s_0\rangle |s_0\rangle \otimes [1, 1, 1, 1] + |s_1\rangle |s_1\rangle \otimes [1, +] |1, +] \).

\(^2\)In \(^1\), the authors need to determine all individual BSCC subspaces, collect those individual BSCC subspaces of the desired parity, and thus check the \( \omega \)-regular properties. To this end, \(^1\) Procedure GetBSCC first compute the direct-sum of BSCC subspaces corresponding to positive eigenvalues and the direct-sum of BSCC subspaces corresponding to negative eigenvalues. If those direct-sums consist of more than one BSCC subspace, the procedure would be respectively applied to the two direct-sums in a recursive manner. The overall complexity is \( O(N^6) \). In our setting, it suffices to compute the direct-sum of all BSCC subspaces, which saves the recursion to complexity \( O(N^5) \). Additionally, determining positive/negative eigenvalues is a typical kind of field operations beyond arithmetic ones (addition, subtraction, multiplication, and division). Obviously, the latter are of lower computational cost.
The BSCC subspaces $\Gamma$ covering all the fixed-points of $\mathcal{F}_{\text{ok}-\text{error}}$ is actually span($|s_0\rangle \otimes |1, 1\rangle$, $|s_1\rangle \otimes |1, +\rangle$). The projection super-operator $\mathcal{P}_\Gamma = \{\mathcal{P}_\Gamma\}$ onto $\Gamma$ is given by the projector $\mathcal{P}_\Gamma = |s_0\rangle\langle s_0| \otimes |1, 1\rangle \langle 1, 1| + |s_1\rangle\langle s_1| \otimes |1, +\rangle \langle 1, +|$; and the projection super-operator $\mathcal{P}_{\Gamma^\perp}$ onto $\Gamma^\perp$ is given by $\mathcal{P}_{\Gamma^\perp} = |s_0\rangle\langle s_0| - \mathcal{P}_\Gamma$. Thereby, the composite super-operator $\mathcal{F}_{\text{ok}-\text{error}} \circ \mathcal{P}_{\Gamma^\perp}$ would have no fixed-point.

**Lemma 5.6.** The identity $\mathcal{P}_{\Phi_1} \circ (\mathcal{F}_{\Phi_1 \wedge \Phi_2})^i = \mathcal{P}_{\Phi_2} \circ (\mathcal{F}_{\Phi_1 \wedge \Phi_2} \circ \mathcal{P}_{\Gamma^\perp})^i$ holds for each $i \geq 0$.

Proof. We will prove it by induction on $i$. When $i = 0$, the identity follows trivially. Assume the identity holds for $i < k$. We proceed to show that it holds for $i = k$. Let $\mathcal{P}_\Gamma = \{|\mathcal{P}_\Gamma\rangle\}$ and $\mathcal{P}_{\Gamma^\perp} = \{|\mathcal{P}_{\Gamma^\perp}\rangle\}$. For any $|\Psi\rangle \in \mathcal{H}_{\text{eq}}$, we have

\[
\mathcal{P}_{\Phi_1} \circ (\mathcal{F}_{\Phi_1 \wedge \Phi_2})^k(|\Psi\rangle \langle \Psi|) = \mathcal{P}_{\Phi_2} \circ (\mathcal{F}_{\Phi_1 \wedge \Phi_2})^k[|\mathcal{P}_\Gamma\rangle + |\mathcal{P}_{\Gamma^\perp}\rangle] \langle \Psi| (|\mathcal{P}_\Gamma\rangle + |\mathcal{P}_{\Gamma^\perp}\rangle)
\]

The fourth equation follows from the facts:

- $|\mathcal{P}_\Gamma\rangle$ is in $\Gamma$, and
- letting $\mathcal{F}$ be a Kraus operator of $\mathcal{F}_{\Phi_1 \wedge \Phi_2}$, then $\mathcal{F}|\mathcal{P}_\Gamma\rangle \langle \Psi|$ is still in $\Gamma$;

and the sixth equation follows from the facts:

- for $k > 1$, $\Gamma$ is orthogonal to $\Gamma^\perp$, and
- for $k = 1$, letting $\mathcal{P}_{\Phi_1 \wedge \Phi_2} = \{|\Phi_1\rangle \otimes \Phi_2\rangle\}$ and $\mathcal{P}_{\Phi_1} = \{|\Phi_1\rangle\}$, then $\Gamma \subseteq \Phi_1 \wedge \Phi_2 \subset \mathcal{H}_{\text{eq}} \subseteq \mathcal{P}_{\Phi_1 \wedge \Phi_2}$. Let $\mathcal{P}_{\Phi_1 \wedge \Phi_2}$ be orthogonal to $\mathcal{P}_{\Phi_1}$. □

We are going to represent $\Lambda(\Phi_1 U \Phi_2)$ using explicit matrices. Recall from [30, Def. 2.2] that, given a super-operator $\mathcal{E} = \{E_\ell : \ell \in [m]\}$, it has the matrix representation

\[
\sum_{\ell \in [m]} E_\ell \otimes E_\ell^*.
\]

where $*$ denotes complex conjugate. Let

- $L^2V(\gamma) := \sum_{i,j \in [n]} (\langle \gamma | j\rangle \langle i | \gamma \rangle)$ be the function that rearranges entries of the linear operator $\gamma$ as a column vector; and

\[
S^2M(\mathcal{E}) := \sum_{\ell \in [m]} E_\ell \otimes E_\ell^*,
\]


- \( V_2L(v) := \sum_{i,j \in [n]} \langle i, j | v | i \rangle | j \) be the function that rearranges entries of the column vector \( v \) as a linear operator.

Here, \( S_2M, L_2V \) and \( V_2L \) are read as “super-operator to matrix”, “linear operator to vector” and “vector to linear operator”, respectively. Then, we have the identities \( V_2L(L_2V(\gamma)) = \gamma \), \( L_2V(\mathcal{E}(\gamma)) = S_2M(\mathcal{E})L_2V(\gamma) \), and \( S_2M(\mathcal{E}_2) \circ \mathcal{E}_1 = S_2M(\mathcal{E}_2)S_2M(\mathcal{E}_1) \). Therefore, all involved super-operator manipulations can be converted to matrix manipulations.

Suppose that all classical states in \( S \) are ordered as \( s_1 < \cdots < s_n \) where \( s_1 \) is the initial one, i.e. \( \Omega = \text{Path}(s_1) \). We notice that for any classical-quantum state \( \rho = \sum_{i \in [n]} | s_i \rangle \langle s_i | \otimes \rho_i \) in \( \mathcal{D}_{\mathcal{H}_{\text{eq}}} \), \( \mathcal{F}_{\Phi_1 \land \cdots \land \Phi_2} \circ \mathcal{P}_{\Gamma} \circ \rho \) and \( \mathcal{P}_{\Gamma} \circ \rho \) keep the mixed form \( \sum_{i \in [n]} | s_i \rangle \langle s_i | \otimes \rho'_i \) for some \( \rho'_i \in \mathcal{D} \). So, we can compressively define the matrix representation of \( \rho \) as a column vector, consisting of \( n \times n \) blocks as entries, in which the \( i \)-th entry is the column vector \( L_2V(\rho_i) \) for \( \rho_i \), i.e. \( M_1 = \sum_{i \in [n]} | i \rangle \otimes L_2V(\rho_i) \).

Let \( \mathcal{F}_{\Phi_1 \land \cdots \land \Phi_3} = \sum_{i,j \in [n]} | s_i \rangle \langle s_i | \otimes Q(s, s_j) = \bigcup_{i,j \in [n]} \bigcup_{i,j} | s_i \rangle \langle s_i | \otimes Q_{i,j,\ell} \gamma \) where \( Q_{i,j,\ell} \) are Kraus operators of \( Q(s, s_j) \) and \( \mathcal{P}_{\Gamma} = \{ | s \gamma \rangle \langle s | \otimes P_{\ell} \} \). Then, \( \mathcal{F}_{\Phi_1 \land \cdots \land \Phi_2} \circ \mathcal{P}_{\Gamma} \) is

\[
\bigcup_{i,j \in [n]} \bigcup_{\ell} \left\{ \sum_{k \in [n]} | s_j \rangle \langle s_k | | s_k \rangle \langle s_l | \otimes Q_{i,j,\ell} P_{\ell} \right\} = \bigcup_{i,j \in [n]} \bigcup_{\ell} \left\{ | s_j \rangle \langle s_i | \otimes Q_{i,j,\ell} P_{\ell} \right\}.
\]

Using it, we further define:

- the matrix representation of \( \mathcal{F}_{\Phi_1 \land \cdots \land \Phi_2} \circ \mathcal{P}_{\Gamma} \) as a square matrix, consisting of \( n^2 \) blocks as entries, in which the \((j,i)\)-th entry is \( \sum_{i,j} Q_{i,j,\ell} P_{\ell} \otimes Q_{i,j,\ell}^* P_{\ell}^* \), i.e.
  \[
  M_2 = \sum_{i,j \in [n]} \sum_{\ell} | \gamma_i \rangle \langle i | \otimes Q_{i,j,\ell} P_{\ell} \otimes Q_{i,j,\ell}^* P_{\ell}^*; \tag{11a}
  \]

- the matrix representation of the projection super-operator \( \mathcal{P}_{\Phi_3} \) as a diagonal matrix, consisting of \( n \) blocks as diagonal entries, in which the \( i \)-th entry is \( I_{\mathcal{H}_{\text{eq}} \otimes \mathcal{H}} \) if the predicate \( s_i \vdash \Phi_2 \) is true, and 0 otherwise, i.e.
  \[
  M_3 = \sum_{i \in [n]} | i \rangle \langle i | \otimes I_{\mathcal{H}_{\text{eq}} \otimes \mathcal{H}} : i \in [n] \land s_i \vdash \Phi_2 \rangle, \tag{11b}
  \]

where \( | i \cdot | \) denotes a multiset.

All these matrix representations are obtained by extending \( \square \) on \( \mathcal{H} \) to the enlarged space \( \mathcal{H}_{\text{eq}} \).

**Lemma 5.7.** The matrix \( I_{\mathcal{H}_{\text{eq}} \otimes \mathcal{H}} - M_2 \) is invertible.

**Proof.** It suffices to show \( M_2 \) has no eigenvalue 1. We assume by contradiction that there is an eigenvector \( v \) of \( M_2 \) associated with eigenvalue 1. That is, \( M_2 v = v \neq 0 \). Then,

\[
\gamma = \sum_{i \in [n]} | s_i \rangle \langle s_i | \otimes V_2L((| i \rangle \otimes I_{\mathcal{H}_{\text{eq}} \otimes \mathcal{H}}) v)
\]

is a linear operator on \( \mathcal{H}_{\text{eq}} \), satisfying \( \mathcal{F}_{\Phi_1 \land \cdots \land \Phi_2} \circ \mathcal{P}_{\Gamma} (\gamma) = \gamma \neq 0 \), while \( \gamma_0 = \gamma + \gamma^\dagger \) also a linear operator on \( \mathcal{H}_{\text{eq}} \), satisfying \( \mathcal{F}_{\Phi_1 \land \cdots \land \Phi_2} \circ \mathcal{P}_{\Gamma} (\gamma_0) = \gamma_0 \neq 0 \). By the definition of \( \Gamma \), we have \( \text{supp}(\gamma_0) \subseteq \Gamma \), and thus \( \mathcal{F}_{\Phi_1 \land \cdots \land \Phi_2} \circ \mathcal{P}_{\Gamma} (\gamma_0) = \mathcal{F}_{\Phi_1 \land \cdots \land \Phi_2}(0) = 0 \neq \gamma_0 \), which contradicts the assumption. \( \square \)
Theorem 5.8 (Matrix representation). Let $M_2$ and $M_3$ be the matrices as defined in (11). Then it is in polynomial time to obtain:

1. the explicit matrix representation of the super-operator $\Delta(X \Phi)$ as $\sum_{s,t} S2M(Q(s, s))$.
2. the explicit matrix representation of $\Delta(\Phi_1 U \Phi_2)$ as
   $$\sum_{i \in [d]} ((\tilde{d} \otimes I_{H^0})M_3(I_{H^0} - M_2^{-1})(I_{H^0} - M_2)^{-1}(1) \otimes I_{H^0}),$$
3. the explicit matrix representation of $\Delta(\Phi_1 U \Phi_2)$ as
   $$\sum_{i \in [d]} ((\tilde{d} \otimes I_{H^0})M_3(I_{H^0} - M_2)^{-1}(1) \otimes I_{H^0}).$$

Proof. The matrix representations directly follow from the semantics of the next formula $X \Phi$, the bounded-until formula $\Delta(\Phi_1 U \Phi_2)$, and the unbounded-until formula $\Delta(\Phi_1 U \Phi_2)$. For complexity, we will analyze them in turn.

1. It is a sum of at most $nd^2$ matrix tensor products, each costs $O(d^4)$. In total, it is in $O(nd^3) \subseteq O(N^6)$.
2. The matrix $I_{H^0} - M_2$ is of dimension $nd^2$. Computing its inverse costs $O(n^3d^6)$. The matrix power $M_2^{k+1}$ amounts to
   $$M_2^{b_2}M_2^{b_1} \cdots M_2^{b_0},$$
   where $(b_1, \ldots, b_1, b_0)$ is the binary code of the positive integer $k+1$ with $l = \lceil \log_2(k+2) \rceil - 1$, i.e. $k+1 = b_0 \cdot 2^0 + b_1 \cdot 2^1 \cdots b_l \cdot 2^l$ with $b_j \in \{0, 1\}$. Computing $M_2^{k+1}$ requires sequentially computing all the factors $M_2^j$ ($j \in [l]$), each of which costs $O(n^3d^6)$; and then computing the product of those factors corresponding to $b_j = 1$, which costs $O(n^3d^6 \log_2(k))$. Other operations are merely a few matrix-vector multiplications over an $nd^2$-dimensional vector space, which costs $O(n^3d^4)$. Totally, it is in $O(n^3d^6 \log_2(k)) \subseteq O(N^6 \log_2(k))$.
3. It is clearly in $O(N^6)$ by the previous analysis.

As a result, the complexity is polynomial time w.r.t. $N = nd$ (reflected in the size of $\mathcal{C}$) and linear time w.r.t. $\log_2(k)$ (reflected in the size of $\phi$).

Example 5.9. Consider the path formulas

$$\phi_1 = \text{true} U \text{ok}, \quad \phi_2 = \text{true} U \text{ok} \downarrow \text{error}, \quad \phi_3 = \text{true} U (\text{ok} \lor \text{error})$$

on the QMC $\mathcal{C}_1$ shown in Example 3.2. For $\phi_4$, the repeated super-operator $F_{\text{ok} \lor \text{error}}$ and the projector $P_1$ whose support covers all its fixed-points have been computed in Example 5.5. Under the order $s_0 < \cdots < s_5$, the matrix representations are calculated as

$$M_2 = \frac{1}{2} \begin{pmatrix} |1\rangle \otimes |1\rangle & |1\rangle \otimes |0\rangle & |0\rangle \otimes |1\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |6\rangle \otimes |1\rangle & |6\rangle \otimes |0\rangle & |0\rangle \otimes |1\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |6\rangle \otimes |2\rangle & |6\rangle \otimes |1\rangle & |1\rangle \otimes |0\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |7\rangle \otimes |1\rangle & |7\rangle \otimes |0\rangle & |0\rangle \otimes |1\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |7\rangle \otimes |2\rangle & |7\rangle \otimes |1\rangle & |1\rangle \otimes |0\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |7\rangle \otimes |3\rangle & |7\rangle \otimes |2\rangle & |2\rangle \otimes |0\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |8\rangle \otimes |1\rangle & |8\rangle \otimes |0\rangle & |0\rangle \otimes |1\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |8\rangle \otimes |2\rangle & |8\rangle \otimes |1\rangle & |1\rangle \otimes |0\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |8\rangle \otimes |3\rangle & |8\rangle \otimes |2\rangle & |2\rangle \otimes |0\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |8\rangle \otimes |4\rangle & |8\rangle \otimes |3\rangle & |3\rangle \otimes |0\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |8\rangle \otimes |5\rangle & |8\rangle \otimes |4\rangle & |4\rangle \otimes |0\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |8\rangle \otimes |6\rangle & |8\rangle \otimes |5\rangle & |5\rangle \otimes |0\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |8\rangle \otimes |7\rangle & |8\rangle \otimes |6\rangle & |6\rangle \otimes |0\rangle & |0\rangle \otimes |0\rangle \end{pmatrix} + \frac{1}{2} \begin{pmatrix} |8\rangle \otimes |8\rangle & |8\rangle \otimes |7\rangle & |7\rangle \otimes |0\rangle & |0\rangle \otimes |0\rangle \end{pmatrix}.$$
in which all eigenvalues of $\mathbf{M}_2$ are $\pm \frac{6}{125} \sqrt{50 + 2 \sqrt{1273}}$, $\pm \frac{6}{125} \sqrt{50 + 2 \sqrt{1273}}$ and 0 of multiplicity 92. Since $\mathbf{M}_2$ has no eigenvalue 1, the matrix inverse $(I_{\mathcal{H}_{qH}} - \mathbf{M}_2)^{-1}$ is well-defined as expected. Finally, the explicit matrix representation $S2M(\Delta(\phi_d))$ of $\Delta(\phi_d)$ is obtained as

$$
\sum_{i=0}^{d} (i \otimes I_{\mathcal{H}_{qH}}) \mathbf{M}_3 (I_{\mathcal{H}_{qH}} - \mathbf{M}_2^{-1}) (I_{\mathcal{H}_{qH}} - \mathbf{M}_2)^{-1} (4 \otimes I_{\mathcal{H}_{qH}})
$$

Similarly, we get other matrix representations

$$
S2M(\Delta(\phi_f)) = \frac{144}{625} [1](3) \otimes I \otimes I \otimes X \otimes X + \frac{81}{625} [1](3) \otimes X \otimes X \otimes X \otimes X + \frac{256}{625} [4](3) \otimes I \otimes I \otimes I \otimes I + \frac{44}{625} [3](3) \otimes I \otimes I \otimes X \otimes X + \frac{16}{625} [1](4) \otimes I \otimes Z \otimes I \otimes Z + \frac{144}{625} [1](4) \otimes Z \otimes I \otimes Z \otimes I + \frac{256}{625} [5](4) \otimes Z \otimes Z \otimes Z \otimes Z.
$$

$\mathbf{M}_3 = [5] \otimes I \otimes I + [6](6) \otimes I \otimes I.$

5.3. Deciding the fidelity-quantifier formula

In the previous subsection, we have constructed an explicit matrix representation $\mathcal{M} := S2M(\mathcal{E})$ for $\mathcal{E} = \Delta(\phi)$ where $\phi$ is the path formula in the fidelity-quantifier formula $\mathcal{H}_{s,t}(\phi)$. Now we present an algebraic approach to compare the (minimum) fidelity $\text{Fid}(\mathcal{E})$ with the threshold $\tau$, so that $s \models \mathcal{H}_{s,t}(\phi)$ can be decided.

We first notice that:
the most common quantum state $|\pm\rangle$ as las, and further encode them as Definition 5.11.

closed fields [27]: composed from polynomial equations and inequalities (as atomic formulas) using logic connectives "\(¬\)"

Definition 5.10. A number $\lambda$ is algebraic, denoted by $\lambda \in \mathbb{A}$, if there is a nonzero $\mathbb{Q}$-polynomial $f(z)$ of least degree, satisfying $f(\lambda) = 0$. Such a polynomial $f(z)$ is called the minimal polynomial $f_\lambda$ of $\lambda$.

Clearly, algebraic numbers widely occur in quantum information, such as the definition of $\psi$.

Since $\psi$.

Roughly speaking, the elements in $\mathcal{H}$ are algebraic numbers for the consideration of computability. Recall that:

Definition 5.11. The theory of real closed fields is a first-order theory $Th(\mathbb{R}; +, \cdot, =, >, 0, 1)$, in which

- the domain is $\mathbb{R}$,
- the functions are addition ‘+’ and multiplication ‘\(\cdot\),
- the predicates are equality ‘=’ and order ‘>, and
- the constants are 0 and 1.

Roughly speaking, the elements in $\mathcal{H}$ are $\mathbb{Q}$-polynomial formulas that are composed from polynomial equations and inequalities (as atomic formulas) using logic connectives “\(-, \land, \lor, \rightarrow, \leftrightarrow\)” and quantifiers “$\forall, \exists$.”

The constraints [12] are the sentences—the formulas whose variables $|\psi\rangle$ are all existentially/universally quantified, i.e. no free variable. We will encode them as $\mathbb{A}$-polynomial formulas, and further encode them as $\mathbb{Q}$-polynomial formulas.

Since $|\psi\rangle\langle\psi|$ is pure, we redefine $|\psi\rangle = \sum_{i\in[d]} x_i |i\rangle$ where $x_i$ ($i \in [d]$) are complex parameters, subject to $\sum_{i\in[d]} x_i x_i^* = 1$. Under the purity, we have

\[
\text{Fid}(\mathcal{E}, |\psi\rangle\langle\psi|) \leq \tau \iff \langle \psi| \mathcal{E}(|\psi\rangle\langle\psi|) |\psi\rangle \leq \tau^2
\]

\[
\equiv \left( \sum_{i\in[d]} x_i^* \langle i| \sum_{j\in[d]} x_j x_j^* |j\rangle \langle j| \right) \left( \sum_{j\in[d]} x_j |j\rangle \langle j| \sum_{i\in[d]} x_i^* \langle i| \right) \leq \tau^2
\]

\[
\equiv \left( \sum_{i,j\in[d]} x_i^* x_j (i, j) \right) \left( \sum_{i,j\in[d]} x_j^* x_i (j, i) \right) \leq \tau^2,
\]
which results in an \( \Lambda \)-polynomial formula. Denote all parameters introduced here by \( \mathbf{x} = (x_i)_{i \in [d]} \). Further, we encode the constraint (12a) as

\[
\zeta_1 \equiv \exists \mathbf{x} : \left[ \sum_{i \in [d]} x_i x_i^* = 1 \land \left( \sum_{i,j \in [d]} x_i^* x_j (i,j) \right) \mathbf{M} \left( \sum_{i,j \in [d]} x_i x_j^* |i,j| \right) \leq \tau^2 \right].
\]  
(14a)

which is the desired \( \Lambda \)-polynomial formula, involving at most

- 2\( d \) real variables (converted from \( d \) complex variables \( \mathbf{x} \)) for expressing \(|\phi|\),
- one quadratic equation for the purity, and
- one quartic inequality for the comparison.

Similarly, the \( \Lambda \)-polynomial formula for encoding the constraint (12b) is

\[
\zeta_2 \equiv \forall \mathbf{x} : \left[ \sum_{i \in [d]} x_i x_i^* = 1 \rightarrow \left( \sum_{i,j \in [d]} x_i^* x_j (i,j) \right) \mathbf{M} \left( \sum_{i,j \in [d]} x_i x_j^* |i,j| \right) \geq \tau^2 \right].
\]  
(14b)

Suppose the input \( \mathcal{E} \) involves real algebraic numbers \( \Lambda = \{ \lambda_j : j \in [e] \} \). Then the \( \Lambda \)-polynomial formulas (14) are named by \( \zeta_1(\Lambda) \) and \( \zeta_2(\Lambda) \), respectively. To effectively tackle them, we resort to the standard encoding of real algebraic number \( \lambda \) that uses minimal polynomial \( f_\lambda \) plus isolation interval \( I_\lambda \), which is given by linear inequalities, like \( z \in I_\lambda \equiv L < z < U \) for some rational endpoints \( L \) and \( U \) of \( I_\lambda \), to distinguish \( \lambda \) from other real roots of \( f_\lambda \). In such a way, to encode each real algebraic number \( \lambda \), we introduce at most

- one real variable \( z \),
- one equation \( f_\lambda = 0 \) of degree \( \deg(f_\lambda) \), and
- two linear inequalities \( z > L \) and \( z < U \) from the isolation interval \( I_\lambda \) of \( \lambda \).

For instance, the aforementioned algebraic number \( 1/\sqrt{2} \) occurring in \(|\phi|\) can be encoded as the unique solution to \( z^2 = \frac{1}{2} \land 0 < z < 1 \).

The \( \Lambda \)-polynomial formulas \( \zeta_1(\Lambda) \) and \( \zeta_2(\Lambda) \) can be rewritten as the \( \mathbb{Q} \)-polynomial ones:

\[
\zeta_1(\Lambda) \equiv \exists \mathbf{z} : \left[ \bigwedge_{j \in [e]} (f_{\lambda_j}(z_j) = 0 \land z_j \in I_{\lambda_j}) \land \zeta_1(\mathbf{z}) \right]
\]  
(15a)

\[
\zeta_2(\Lambda) \equiv \forall \mathbf{z} : \left[ \bigwedge_{j \in [e]} (f_{\lambda_j}(z_j) = 0 \land z_j \in I_{\lambda_j}) \rightarrow \zeta_2(\mathbf{z}) \right],
\]  
(15b)

where \( \mathbf{z} = (z_j)_{j \in [e]} \) are real variables introduced to symbolize \( \Lambda \). Note that the existential quantifier \( \exists \mathbf{z} \) and the universal quantifier \( \forall \mathbf{z} \) can be mutually converted here, since for each \( j \in [e] \), there is a unique solution (i.e. \( \lambda_j \)) to the subformula \( f_{\lambda_j}(z_j) = 0 \land z_j \in I_{\lambda_j} \) by the standard encoding of \( \lambda_j \).

Finally, applying the existential theory of the reals \([3\text{, Thm. 13.13}]\), we obtain:

**Theorem 5.12 (Decidability).** It is in exponential time to decide the fidelity-quantifier formula \( \overline{\mathcal{R}}_{\mathcal{F}}(\phi) \).
Proof. It suffices to show that the formulating subprocedure is in polynomial time, and that the deciding subprocedure is in exponential time.

The encoding on the purity is plainly in $O(d)$. Encoding the left hand side of the comparison (e.g., the formula (13)) involves a few matrix-vector multiplications over a $d^2$-dimensional vector space, which costs $O(d^6)$. Thus encoding the polynomial formulas (15) is in $O(d^4)$, which means that the formulating subprocedure is in polynomial time.

Then we tackle the deciding subprocedure, which invokes the following Algorithm 2 on the formulas (15). Technically, the formulas (15) have

- a block of $2d + e$ real variables $x$ and $z$ quantified all by ‘∃’ for (15a) or all by ‘∀’ for (15b), and
- at most $C = 2 + 3e$ distinct polynomials of degree at most $D = \max(4, \max_{j \in \{e\}} \deg(f_{ij}))$.

Thereby, the complexity is in $C^{2d+e+1}D^{O(2d+e)}$, an exponential hierarchy. □

Algorithm 2 Existential Theory of the Reals [5, Thm. 13.13].

```
true/false ← QE(Qx : F(x))
```

**Input:** $Qx : F(x)$ is a quantified polynomial formula, in which

- $x$ is a block of $k$ real variables, which is quantified by $Q \in \{\forall, \exists\}$,
- each atomic formula in $F$ is in the form $p \sim 0$ where $\sim \in \{<, \leq, =, \geq, >, \neq\}$,
- all distinct polynomials $p$, regardless of a constant factor, extracted from those atomic formulas $p \sim 0$ form a polynomial collection $\mathbb{P}$,
- $C$ is the cardinality of $\mathbb{P}$, and
- $D$ is the maximum degree of the polynomials in $\mathbb{P}$.

**Output:** $true/false$ is the truth of $Qx : F(x)$.

**Complexity:** $C^{k+1}D^{O(k)}$.

There are many packages that have implemented Algorithm 2, such as REDUCE (a.k.a. REDLOG [10]) and Z3 [8].

**Example 5.13.** Consider the events that

1. “the IP address is properly configured”,
2. “the IP address is properly configured within 15 steps”,
3. “the IP address is properly or wrongly configured”, and
4. “the IP address is properly or wrongly configured within 15 steps”

on the QMC $\mathcal{G}_1$ shown in Example 3.2 which are specified by the path formulas $\phi_1$ through $\phi_4$ in Example 5.9 respectively. For $\phi_1 = true \cup 15(ok \lor error)$, the explicit matrix representation $\mathbb{M}$ of $\mathbb{M}(\phi_1)$ has been obtained. Now we are to decide the fidelity-quantifier formula $\mathbb{M}_{\leq \tau}(\phi_4)$.

After introducing the real variables $\mu = \mathcal{R}(x)$ and $\nu = \mathcal{I}(x)$ where $x = (x_i)_{i \in \{a\}}$ encodes the pure state $|\psi\rangle\langle\psi|$, we have the desired polynomial formula
\[ \{\mu, \nu\} : [\mu_1^2 + \nu_1^2 + \mu_2^2 + \nu_2^2 + \mu_3^2 + \nu_3^2 + \mu_4^2 + \nu_4^2 = 1 \land \frac{337}{1000} \nu_1^4 + 331840704685856836307974101662 \nu_1^2 + 5017502987841674533676457823331 \nu_2^4 + 14 + \frac{337}{1000} \nu_3^4 + 14 + \frac{337}{1000} \nu_4^4 + \cdots] 
\]

By Reduce \cite{10}, the fidelity-quantifier formula \( \tilde{\nu}_{567/100}(\phi_4) \) is decided to be true while \( \tilde{\nu}_{567/100}(\phi_4) \) is false. In other words, \( \text{Fid}(\Lambda(\phi_4)) \) is in \( \tilde{\nu}_{567/100}(\phi_4) \), which entails that at least 67% of the original MAC and proper IP addresses at \( s_3 \) would be delivered at the terminal \( s_4 \) or \( s_5 \) within 15 steps through the noisy channel \( C_1 \). Besides, by \cite{12}, we can compute that it has probability at least \( \frac{337}{1000} \) to reach \( s_4 \) or \( s_5 \) within 15 steps, whose square-root can be proven to be an upper bound of the fidelity, i.e. \( \frac{337}{1000} \), no lower bound. So it is less precise than ours in characterizing the similarity degree of the two MAC addresses.

For the formulas \( \phi_1 \) and \( \phi_2 \), we have that both \( \tilde{\nu}_{567/100}(\phi_1) \) and \( \tilde{\nu}_{567/100}(\phi_2) \) hold, since there are some pure states, whose support falls into the BSCC subspaces w.r.t. \( \tau \). For instance, \( [s_3]([s_3] \otimes [1, 1, 1]) \) is transformed to \( [s_4]([s_4] \otimes [Q(s_3, s_4)]([1, 1, 1])) \) to \( [s_3]([s_3] \otimes [1, 1, 1]) \), whose support itself forms a BSCC subspace; and to \( [s_4]([s_4] \otimes [Q(s_3, s_4)]([1, 1, 1])) \) to \( [s_3]([s_3] \otimes [1, 1, 1]) \), whose support falls into the BSCC subspace span([0]) \( \otimes [1, 1, 1] \), \( [s_1] \otimes [1, 1, 1] \). Besides, we have that both \( \tilde{\nu}_{567/100}(\phi_1) \) and \( \tilde{\nu}_{567/100}(\phi_2) \) hold, as the bounded-until formula approaches the unbounded-until one.

Remark 5.14. When the initial density operator \( \rho \) is given and all the entries in the Kraus operators of \( Q(s, t) \) with \( s, t \in S \) are rational, it would be in polynomial time to decide \( (s, \rho) \models \tilde{\nu}_{\tau}([\phi]) \), since the time-consuming quantifier elimination is saved then. It is consistent with the existing work \cite{10}.

Implementation. We have implemented the presented method on the platform Mathematica, incorporated with the package Reduce \cite{10}. Using caching mechanism, we divide the whole computation procedure into two subprocedures:

1. the synthesizing subprocedure to prepare information about the given QMC and QCTL formula, including quantum state information, matrix representations of transition superoperators, and removal of the direct-sum of all BSCC subspaces; and
2. the deciding subprocedure for fidelity-quantifier formulas.

Thus we can for instance ensure good interactivity in specific situations. Under a PC with Intel Core i7-6700 CPU and 8 GB RAM, the overall performance of our running examples is acceptable: the total time consumption is within a few seconds; the synthesizing subprocedure
consumes nearly 30 MB memory, and besides that, the deciding subprocedure consumes at most 50 MB. Finally, we have to address that the fidelity computation for the QMC with a concrete initial classical–quantum state is always much efficient (usually within 1 second); while the fidelity computation for the QMC with a parametric initial classical–quantum state may be inefficient, since in the worst case the quantifier elimination is exponential time. Detailed calculation procedure is available at https://github.com/melonysuga/PaperFidelityExamples-.git.

6. Conclusion

In this paper, we introduced a quantum analogy of computation tree logic (QCTL), which consists of state formulas and path formulas. A model checking algorithm was presented over the quantum Markov chains (QMCs). We gave a simple polynomial time procedure that could remove all fixed-points w.r.t. a super-operator. We then synthesized the super-operators of path formulas using explicit matrix representations, and decided the fidelity-quantifier formulas by a reduction to quantifier elimination in the existential theory of the reals. Finally, the QCTL formulas were shown to be decidable in exponential time.

We believe that the proposed method could be extended to:

- synthesize the SOVM for the general multiphase until formula \( \Phi_1 U^i \Phi_2 U^{j_2} \cdots U^{j_{k-1}} \Phi_k \) with proper time intervals \( I_i \), as in [29];
- synthesize the SOVM for the conjunction \( \phi_1 \land \phi_2 \), so that the conditional fidelity, similar to conditional probability [2, 13], could be established;
- synthesize the SOVM for the negation \( \neg \phi \), so that the safety property \( \Box \Phi = \neg (\text{true} U \neg \Phi) \) could be analyzed; and
- decide the analogy of SOVM-quantifier formula over parametric QMCs. The positive-operator valued measure (POVM) would be a key tool to attack it.

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