## Model checking quantum Markov chains

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#### Outline



- 2 Basic notions from quantum information theory
- 3 Quantum Markov chain
- Quantum computation tree logic
- **5** Algorithm





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#### 1 Motivation

- 2 Basic notions from quantum information theory
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- 5 Algorithm
- 6 Summary



## **Motivation**

- Quantum mechanics is highly counterintuitive; flaws and errors creep in during the design of quantum programs and quantum protocols.
- So, it is indispensable to develop techniques of verifying and debugging quantum systems.



#### Model checking

- Model-checking is one of the dominant techniques for verification of classical hardware as well as software systems.
- It has proved mature as witnessed by a large number of successful industrial applications.
- Quantum model checking???



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# Probability Theory v.s. Quantum Information Theory

Binary Random Varable X:

$$X = 0$$
 or  $X = 1$ 

#### Quantum bit:

Unit vector in a 2D Hilbert space  $|\phi\rangle = a_0|0\rangle + a_1|1\rangle$ ,  $a_i \in C$ ,  $|a_0|^2 + |a_1|^2 = 1$ 



## Probability Theory v.s. Quantum Information Theory

Evolution: Stochastic Matrices

Evolution: Unitary Matrices

Preserve  $l_1$ -norm  $p' = S \cdot p$ 

$$\left(\begin{array}{cc} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{array}\right) \left(\begin{array}{c} p_0 \\ p_1 \end{array}\right) = \left(\begin{array}{c} \frac{1}{2} \\ \frac{1}{2} \end{array}\right)$$

Preserve *l*<sub>2</sub>-norm  

$$\begin{aligned} |\phi'\rangle &= U \cdot |\phi\rangle \\ \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}(a_0 + a_1) \\ \frac{1}{\sqrt{2}}(a_0 - a_1) \end{pmatrix} \end{aligned}$$



# Probability Theory v.s. Quantum Information Theory

Observation:

$$\Pr(X = b) = p_b,$$
  
$$p_b \in [0, 1]$$

#### Measurement:

A measurement of  $|\phi\rangle$  according to a Hermitian operator  $M = \sum_i \lambda_i |b_i\rangle \langle b_i|$  is a projection onto the orthonormal vectors  $|b_i\rangle$ , and  $\Pr[\text{outcome is } \lambda_i] = |\langle \phi | b_i \rangle|^2$ .

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#### **Density operators**

• Mixed state: Classical distribution over (pure) quantum states.

$$ho = \left\{ egin{array}{ll} |\phi_1
angle, & ext{with probability } p_1 \ dots & dots \ |\phi_k
angle, & ext{with probability } p_k \ ec{ ext{Ensemble:}} & \{p_i: |\phi_i
angle\}. \end{array} 
ight.$$

- Density operator:  $ho=\sum_{i=1}^k 
  ho_i |\phi_i
  angle \langle \phi_i|$  (hermitian, trace 1, positive)
  - Contains all information about the state.
  - Different ensembles can have the same density operator.



#### **Density operators**

• Different ensembles can have the same density operator.

$$\begin{cases} \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle), & \text{w.p.} \quad \frac{1}{2} \\ |0\rangle, & \text{w.p.} \quad \frac{1}{2} \end{cases} = \\ \begin{cases} \frac{\sqrt{3}}{2}|0\rangle - \frac{1}{2}|1\rangle, & \text{w.p.} \quad \frac{1}{\sqrt{3}} \\ |0\rangle, & \text{w.p.} \quad \frac{3}{4}(1 - \frac{1}{\sqrt{3}}) \\ |1\rangle, & \text{w.p.} \quad \frac{1}{4}(1 - \frac{1}{\sqrt{3}}) \end{cases} = \begin{pmatrix} \frac{3}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{1}{4} \end{pmatrix}$$



#### Super-operators and Kraus theorem

- Super-operators: (special) mapping from density operators to density operators.
- Kraus representation theorem: A map  $\mathcal E$  is a super-operator if and only if

$$\mathcal{E}(\rho) = \sum_{i=1}^{d} E_i \rho E_i^{\dagger}$$

for some set of matrices  $\{E_i, i=1,\ldots,d\}$  with  $\sum_i E_i^{\dagger} E_i \leq I$ .

- Special case:
  - Unitary transformation:  $ho o U 
    ho U^{\dagger}$
  - Measurement with outcome  $i: \rho \to |b_i\rangle\langle b_i|\rho|b_i\rangle\langle b_i|$

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• Measurement with reading outcome:  $\rho \rightarrow \sum_i |b_i\rangle \langle b_i | \rho | b_i \rangle \langle b_i |$ 

#### Matrix representation of super-operators

Let  $\mathcal{E} = \{E_i : i \in I\}$  be a super-operator. The matrix representation of  $\mathcal{E}$  is defined as

$$M_{\mathcal{E}} = \sum_{i \in I} E_i \otimes E_i^*.$$

Here the complex conjugate is taken according to the orthonormal basis  $\{|k\rangle : k \in K\}$ . It is easy to check that  $M_{\mathcal{E}}$  is independent of the choice of orthonormal basis and the Kraus operators  $E_i$ .



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#### Markov chains

A Markov chain (MC) is a tuple (S, P) where

- S is a countable set of states;
- P:S imes S o [0,1] such that for each  $s\in S$ ,

$$\sum_{t\in S} P(s,t) = 1,$$

or equivalently,  $P(s, \cdot)$  is a probabilistic distribution over S.



## Quantum Markov chains

( <i>S</i> , <i>P</i> )	$\Rightarrow$	$(\mathcal{H},\mathcal{E})$
Set <i>S</i>	$\Rightarrow$	Hilbert space ${\cal H}$
Prob. distributions	$\Rightarrow$	Density operators
$P: \textit{Dist}(S) \rightarrow \textit{Dist}(S)$	$\Rightarrow$	$\mathcal{E}:\mathcal{D}(\mathcal{H})\to\mathcal{D}(\mathcal{H})$



#### Obstacles for model checking quantum system

- The set of all possible quantum states,  $\mathcal{H}$ , is a continuum, even when it is finite dimensional.
- The techniques of classical model checking, which normally work for finite state spaces, cannot be applied directly.



#### In this talk, we propose...

- A super-operator weighted Markov chain model which aims at providing finite models for general quantum programs and quantum communication protocols.
- A quantum extension QCTL of the logic PCTL to describe properties we are interested in for QMCs.
- An algorithm to model check logic formulas in QCTL against a QMC model.



### Some more notations

## Let $\mathcal{SO}(\mathcal{H})$ be the set of super-operators on $\mathcal{H},$ ranged over by $\mathcal{E},\mathcal{F},\cdots.$

#### Definition

Let  $\mathcal{E}, \mathcal{F} \in \mathcal{SO}(\mathcal{H}).$ 

- $\mathcal{E} \sqsubseteq \mathcal{F}$  if for any  $\rho \in \mathcal{D}(\mathcal{H})$ ,  $\mathcal{F}(\rho) \mathcal{E}(\rho)$  is positive semi-definite;
- $\textbf{2} \ \mathcal{E} \lesssim \mathcal{F} \text{ if for any } \rho \in \mathcal{D}(\mathcal{H}), \, \mathrm{tr}(\mathcal{E}(\rho)) \leq \mathrm{tr}(\mathcal{F}(\rho)).$

Let  $\approx$  be  $\leq \cap \geq$ ; it is obviously an equivalence relation.



#### Some notations

#### Let

$$\mathcal{SI}(\mathcal{H}) = \{\mathcal{E} \in \mathcal{SO}(\mathcal{H}): \mathcal{E} \lesssim \mathcal{I}_{\mathcal{H}}\}$$

be the 'quantum' correspondence of the unit interval  $\left[0,1\right]$  for real numbers.



#### **Quantum Markov chains**

A super-operator weighted Markov chain, or quantum Markov chain (QMC), over  $\mathcal{H}$  is a tuple (*S*, **Q**, *AP*, *L*), where

- S is a countable set of states;
- $\mathbf{Q}: S \times S \to \mathcal{SI}(\mathcal{H})$  such that for each  $s \in S$ ,  $\sum_{t \in S} \mathbf{Q}(s, t) \eqsim \mathcal{I}_{\mathcal{H}}$ ,
- AP is a finite set of atomic propositions;
- L is a mapping from S to  $2^{AP}$ .

A classical Markov chain may be viewed as a degenerate quantum Markov chain in which all super-operators appear in the transition matrix have the form  $p\mathcal{I}_{\mathcal{H}}$  for some  $0 \le p \le 1$ .



#### Example: quantum loop

A simple quantum loop program goes as follows:

$$\begin{array}{rrrr} \mathit{l}_0 & : & q := \mathcal{F}(q) \\ \mathit{l}_1 & : & \textbf{while } \mathit{M}[q] \ \textbf{do} \\ \mathit{l}_2 & : & q := \mathcal{E}(q) \\ \mathit{l}_3 & : & \textbf{od} \end{array}$$

where  $M = \lambda_0 |0\rangle \langle 0| + \lambda_1 |1\rangle \langle 1|$ .



## Example: quantum loop



Here  $\mathcal{E}_q^0 = \{|0
angle_q \langle 0|\}$  and  $\mathcal{E}_q^1 = \{|1
angle_q \langle 1|\}.$ 



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The syntax of quantum computation tree logic (QCTL) is as follows:

$$\begin{split} \Phi & ::= & a \mid \neg \Phi \mid \Phi \land \Psi \mid \mathbb{Q}_{\sim \mathcal{E}}[\psi] \\ \psi & ::= & \mathbf{X} \Phi \mid \Phi \mathbf{U} \Psi \end{split}$$

where a is an atomic proposition,  $\sim \in \{\leq, \geq\}$ , and  $\mathcal{E} \in \mathcal{SI}(\mathcal{H})$ . We call  $\Phi$  a state formula and  $\psi$  a path formula.



Let  $\mathcal{M} = (S, \mathbf{Q}, AP, L)$ . The satisfaction relation  $\models$  is defined inductively: for any state  $s \in S$ ,

$$\begin{array}{ccc} s \models a & \text{iff} & a \in L(s) \\ s \models \neg \Phi & \text{iff} & s \not\models \Phi \\ s \models \Phi \land \Psi & \text{iff} & s \models \Phi \text{ and } s \models \Psi \end{array}$$

and for any path  $\pi \in \textit{Path}^\mathcal{M}(s)$ ,

$$\begin{split} \pi &\models \mathbf{X} \Phi \quad \text{iff} \quad \pi(1) \models \Phi \\ \pi &\models \Phi \mathbf{U} \Psi \quad \text{iff} \quad \exists i \in \mathbb{N}. (\pi(i) \models \Psi \land \forall j < i. (\pi(j) \models \Phi)). \end{split}$$



#### Finally,

$$s \models \mathbb{Q}_{\sim \mathcal{E}}[\psi]$$
 iff  $\mathcal{Q}^{\mathcal{M}}(s,\psi) \sim \mathcal{E}$ 

where

$$Q^{\mathcal{M}}(s,\psi) = Q_s(\{\pi \in \mathsf{Path}^{\mathcal{M}}(s) \mid \pi \models \psi\}).$$

#### But how to define $Q_s$ ?



#### Super-operator valued measures

Let  $(\Omega, \Sigma)$  be a measurable space; that is,  $\Omega$  is a non-empty set and  $\Sigma$  a  $\sigma$ -algebra over  $\Omega$ . A function  $\Delta : \Sigma \to S\mathcal{I}(\mathcal{H})$  is said to be a super-operator valued measure (SVM for short) if  $\Delta$  satisfies the following properties:

- ②  $\Delta(\biguplus_i A_i) ≂ \sum_i \Delta(A_i)$  for all pairwise disjoint and countable sequence  $A_1$ ,  $A_2$ , ... in  $\Omega$ .

We call the triple  $(\Omega, \Sigma, \Delta)$  a (super-operator valued) measure space.



#### Properties of super-operator valued measures

- Let  $(\Omega, \Sigma, \Delta)$  be a measure space. Then

  - $(\mathbf{A}^{c}) + \Delta(\mathbf{A}) \eqsim \mathcal{I}_{\mathcal{H}};$
  - S for any A, A' ∈ Σ, if A ⊆ A' then  $\Delta(A) \lesssim \Delta(A')$ ;

• for any sequence  $A_1, A_2, \ldots$  in  $\Sigma$ ,

- if  $A_1 \subseteq A_2 \subseteq \ldots$ , then there exists a sequence  $\mathcal{E}_1 \sqsubseteq \mathcal{E}_2 \sqsubseteq \ldots$  in  $\mathcal{SI}(\mathcal{H})$  such that for any *i*,  $\Delta(A_i) \eqsim \mathcal{E}_i$ , and  $\Delta(\bigcup_{i>1} A_i) = \lim_{i \to \infty} \mathcal{E}_i$ .
- if  $A_1 \supseteq A_2 \supseteq \ldots$ , then there exists a sequence  $\mathcal{E}_1 \sqsupseteq \mathcal{E}_2 \sqsupseteq \ldots$  in  $\mathcal{SI}(\mathcal{H})$  such that for any *i*,  $\Delta(A_i) \eqsim \mathcal{E}_i$ , and  $\Delta(\bigcap_{i \ge 1} A_i) = \lim_{i \to \infty} \mathcal{E}_i$ .



#### SVM for a QMC

Fix a state  $s \in S$ .

- Sample space  $\Omega = Path^{\mathcal{M}}(s)$ .
- Let the cylinder set  ${\it Cyl}(\widehat{\pi})\subseteq {\it Path}^{\mathcal{M}}(s)$  be defined as

$${\it Cyl}(\widehat{\pi})=\{\pi\in {\it Path}^{\mathcal{M}}({\it s}):\widehat{\pi} \text{ is a prefix of }\pi\};$$

that is, the set of all infinite paths with prefix  $\widehat{\pi}.$ 

•  $\sigma$ -algebra over  $\Omega$ :

$$\Sigma^{s} = \sigma(\{Cyl(\widehat{\pi}) : \widehat{\pi} \in Path_{fin}^{\mathcal{M}}(s)\})$$

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#### SVM for QMCs

• For any finite path  $\widehat{\pi} = s_0 \dots s_n \in Path_{fin}^{\mathcal{M}}(s)$ , we define the super-operator

$$\mathbf{Q}(\widehat{\pi}) = \left\{ \begin{array}{ll} \mathcal{I}_{\mathcal{H}}, & \text{if } n = 0; \\ \mathbf{Q}(s_{n-1}, s_n) \cdots \mathbf{Q}(s_0, s_1), & \text{otherwise.} \end{array} \right.$$

• Let a mapping  $Q_s$  be defined by letting  $Q_s( arnow ) = 0_{\mathcal{H}}$  and

$$Q_s(Cyl(\hat{\pi})) = \mathbf{Q}(\hat{\pi}). \tag{1}$$



## Extend Q<sub>s</sub> to a SVM

#### Theorem

The mapping  $Q_s$  can be extended to a SVM on the  $\sigma$ -algebra  $\Sigma^s$ . Furthermore, this extension is unique up to the equivalence relation  $\overline{\sim}$ .

Remark: The main tool we use to prove this theorem is the Kluvanek's generalisation of the Carathéodory-Hahn extension theorem from vector measure theory.



#### Theorem

For each path formula  $\psi$  and each state s in a QMC  $\mathcal{M},$  the set

$$\{\pi \in \mathsf{Path}^{\mathcal{M}}(s) \mid \pi \models \psi\}$$

is measurable.



#### Back to the example



Let  $\Diamond \Psi \equiv tt \mathbf{U} \Psi$ . The QCTL formula  $\mathbb{Q}_{\geq \mathcal{E}}[\Diamond I_3]$  asserts that the probability that the loop program terminates is lower bounded by  $\mathcal{E}$ . That is, for any initial quantum state  $\rho$ , the termination probability is not less than  $tr(\mathcal{E}(\rho))$ .

In particular, the property that it terminates everywhere described as  $\mathbb{Q}_{\geq \mathcal{I}_{\mathcal{H}}}[\Diamond I_3]$ .



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#### Model checking

Given a state *s* in a qMC  $\mathcal{M} = (S, \mathbf{Q}, AP, L)$  and a state formula  $\Phi$  expressed in QCTL, model checking if  $s \models \Phi$  is essentially to determine whether *s* belongs to the satisfaction set  $Sat(\Phi) = \{s \in S : s \models \Phi\}$  which is defined inductively as follows:

$$\begin{array}{lll} \mathsf{Sat}(\mathsf{a}) &=& \{\mathsf{s} \in \mathsf{S} : \mathsf{a} \in \mathsf{L}(\mathsf{s})\}\\ \mathsf{Sat}(\neg \Psi) &=& \mathsf{S} \backslash \mathsf{Sat}(\Psi)\\ \mathsf{Sat}(\Psi \land \Phi) &=& \mathsf{Sat}(\Psi) \cap \mathsf{Sat}(\Phi)\\ \mathsf{Sat}(\mathbb{Q}_{\sim \mathcal{E}}[\psi]) &=& \{\mathsf{s} \in \mathsf{S} : \mathcal{Q}^{\mathcal{M}}(\mathsf{s},\psi) \sim \mathcal{E}\}. \end{array}$$

 $\texttt{Recall:} \quad Q^{\mathcal{M}}(s,\psi) = Q_s(\{\pi \in \textit{Path}^{\mathcal{M}}(s) \ | \ \pi \models \psi\})$ 



#### Case 1: $\psi = X\Phi$

By definition,  $\{\pi \in Path^{\mathcal{M}}(s) : \pi \models \mathbf{X}\Phi\} = \biguplus_{t \in Sat(\Phi)} Cyl(st)$ . Thus

$$\begin{array}{lcl} Q^{\mathcal{M}}(s,\mathbf{X}\Phi) & = & Q_s\left(\biguplus_{t\in Sat(\Phi)} Cyl(st)\right) \eqsim \sum_{t\in Sat(\Phi)} Q_s(Cyl(st)) \\ & = & \sum_{t\in Sat(\Phi)} \mathbf{Q}(s,t). \end{array}$$

This can be calculated easily since by the recursive nature of the definition, we can assume that  $Sat(\Phi)$  is already known.



#### Case 2: $\psi = \Phi U \Psi$

In this case, after some calculation, we get the equation system

$$Q^{\mathcal{M}}(s, \Phi \mathbf{U} \Psi) \approx \begin{cases} \mathcal{I}_{\mathcal{H}}, & \text{if } s \in Sat(\Psi); \\ \mathbf{0}_{\mathcal{H}}, & \text{if } s \notin Sat(\Phi) \cup Sat(\Psi); \\ \sum_{t \in S} Q^{\mathcal{M}}(t, \Phi \mathbf{U} \Psi) \mathbf{Q}(s, t), & \text{if } s \in Sat(\Phi) \backslash Sat(\Psi). \end{cases}$$

Then for each  $s \in Sat(\Phi) \setminus Sat(\Psi)$ ,

$$Q^{\mathcal{M}}(s, \Phi \mathbf{U} \Psi) \approx \sum_{t \in \mathit{Sat}(\Phi) \backslash \mathit{Sat}(\Psi)} Q^{\mathcal{M}}(t, \Phi \mathbf{U} \Psi) \mathbf{Q}(s, t) + \sum_{t \in \mathit{Sat}(\Psi)} \mathbf{Q}(s, t).$$



Let 
$$S' = Sat(\Phi) \setminus Sat(\Psi)$$
. For any  $s \in S'$ ,  
 $Q^{\mathcal{M}}(s, \Phi \mathbf{U}\Psi) \approx \sum_{t \in S'} Q^{\mathcal{M}}(t, \Phi \mathbf{U}\Psi) \mathbf{Q}(s, t) + \sum_{t \in Sat(\Psi)} \mathbf{Q}(s, t)$ .

Let

$$\mathcal{T} = \left[\mathbf{Q}(t,s)\right]_{s,t\in S'}$$

and

$$\mathcal{G} = \left[\sum_{t \in Sat(\Psi)} \mathbf{Q}(s, t)\right]_{s \in S'}.$$

Then the required row vector  $(Q^{\mathcal{M}}(s, \Phi \mathbf{U}\Psi))_{s \in S'}$  is equivalent to the fixed point of the function

$$f(X) = X\mathcal{T} + \mathcal{G}.$$

## A theorem

#### Theorem

#### Let

$$f(X) = X\mathcal{T} + \mathcal{G}$$

be defined above. Then

- f(X) has the least fixed point, denoted by E<sup>0</sup>, in SI(H)<sup>|S'|</sup> under the order ⊑;
- ② Given any  $\mathcal{E} \in S\mathcal{I}(\mathcal{H})$  and  $1 \leq i \leq |S'|$ , it can be decided whether  $\mathcal{E} \sim \mathcal{E}_i^0$ , ~ ∈{≲, ≥}, in time  $O(n^2d^4)$  where  $d = dim(\mathcal{H})$  is the dimension of  $\mathcal{H}$  and n = |S'|.



#### Back to the example again

We check the property  $\mathbb{Q}_{\geq \mathcal{E}}[\Diamond I_3] = \mathbb{Q}_{\geq \mathcal{E}}[\text{tt}\mathbf{U}I_3]$  when  $\mathcal{F} = \{|+\rangle\langle i|: i = 0, 1\}, \ \mathcal{E}^i = \{|i\rangle\langle i|\}, \ i = 0, 1, \text{ and } \mathcal{E} = \mathcal{X}.$ 



We first calculate that  $Sat(I_3) = \{I_3\}$  and  $Sat(tt) = \{I_0 \land I_1 \land I_3\}$ 

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#### Back to the example again



$$\begin{array}{rcl} Q^{\mathcal{M}}(l_{0},\Diamond \ l_{3}) &=& Q^{\mathcal{M}}(l_{1},\Diamond \ l_{3})\mathcal{F} \\ Q^{\mathcal{M}}(l_{1},\Diamond \ l_{3}) &=& Q^{\mathcal{M}}(l_{2},\Diamond \ l_{3})\mathcal{E}^{1} + \mathcal{E}^{0} \\ Q^{\mathcal{M}}(l_{2},\Diamond \ l_{3}) &=& Q^{\mathcal{M}}(l_{1},\Diamond \ l_{3})\mathcal{E} \end{array}$$



#### Example

We calculate that for i = 0, 1, 2,

$$Q^{\mathcal{M}}(l_i, \Diamond \ l_3) = Set^0$$
  
where  $Set^0 = \{|0
angle\langle 0|, |0
angle\langle 1|\} \equiv \mathcal{I}$ , and so  
 $l_i \models \mathbb{Q}_{\gtrsim \mathcal{E}}[\Diamond \ l_3]$ 

for any  $\mathcal{E} \lesssim \mathcal{I}$ .



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#### **Topics for further studies**

- Tools to implement the model checking algorithm.
- Model checking quantum properties.
- Check security of physically implemented quantum cryptographic systems.



## Thank you!

## Questions or Comments?

