Model Checking Quantum Systems — A Survey

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Abstract—This article discusses the essential difficulties in developing model-checking techniques for quantum systems that are never present in model checking classical systems. It further reviews some early researches on checking quantum communication protocols as well as a new line of researches pursued by the authors and their collaborators on checking general quantum systems, applicable to both physical systems and quantum programs.

I. INTRODUCTION

We are currently in the midst of a second quantum revolution: transition from quantum theory to quantum engineering [16]. The aim of quantum theory is to find fundamental rules that govern the physical systems already existing in nature. Instead, quantum engineering intends to design and implement new systems (machines, devices, etc) that do not exist before to accomplish some desirable tasks, based on quantum theory. Active areas of quantum engineering includes quantum computing, quantum cryptography, quantum communication, quantum sensing, quantum simulation, quantum metrology and quantum imaging.

Experiences in today's engineering indicate that it is not guaranteed that a human designer completely understands the behaviours of the systems she/he designed, and a bug in her/his design may cause some serious problems and even disasters. So, correctness, safety and reliability of complex engineering systems have attracted wide attention and have been systematically studied in various engineering fields. In particular, in the last four decades, computer scientists have developed various verification techniques for the correctness of both hardware and software as well as the security of communication protocols.

A. Second Quantum Revolution Requires New Verification Techniques

As is well-known, human intuition is much better adapted to the classical world than the quantum world. This implies that human engineers will commit many more faults in designing and implementing complex quantum systems such as quantum computer hardware and software and quantum communication protocols. Thus, correctness, safety and reliability problems will be even more critical in quantum engineering than in today's engineering. However, due to the essential differences between the classical and quantum worlds, verification techniques developed for classical engineering systems cannot be directly used to quantum systems. Novel verification techniques will be indispensable for the coming era of quantum engineering and quantum technology [12].

B. Model Checking Techniques for Classical Systems

Model-checking is an effective automated technique that checks whether a desired property is satisfied by a system, e.g. a computing or communication system. The properties that are checked are usually specified in a logic, in particular, temporal logic; typical properties are deadlock freedom, invariants, safety, request-response properties. The systems under checking are mathematically modelled as e.g. (finite-state) automata, transition systems, Markov chains and Markov decision processes [13, 4].

Model-checking has become one of the dominant techniques for verification of computer (hardware and software) systems 30 years after its inception. Many industrial-strength systems have been verified by employing model-checking techniques. Recently, it has also successfully been used in systems biology; see [31] for example.

With quantum engineering and quantum technology being emerging, a question then naturally arises: is it possible and how to use model-checking techniques to verify correctness and safety of quantum engineering systems?

C. Difficulty in Model Checking Quantum Systems

Unfortunately, it seems that the current model-checking techniques cannot be directly applied to quantum systems because of some essential differences between the classical world and the quantum world. To develop model-checking techniques for quantum systems, the following three problems must be systematically addressed:

- **System modelling and property specification**: The classical system modelling method cannot be used to describe the behaviours of quantum systems, and the classical specification language is not suited to formalise the properties of quantum systems to be checked. So, we need to carefully and clearly define a conceptual framework in which we can properly reason about quantum systems, including formal models of quantum systems and formal description of temporal properties of quantum systems.

- **Quantum measurements**: Model-checking is usually applied to check long-term behaviours of the systems. But to check whether a quantum system satisfies a certain property at a time point, one has to perform a quantum
measurement on the system, which can change the state of the system. This makes studies of the long-term behaviours of quantum systems much harder than that of classical systems [22], [10], [11].

- **Algorithms**: The state spaces of the classical systems that model-checking algorithms can be applied to are usually finite or countably infinite. However, the state spaces of quantum systems are inherently continuous even when they are finite-dimensional. In order to develop algorithms for model-checking quantum systems, we have to exploit some deep mathematical properties of the systems so that it suffices to examine only a finite number of (or at most countably infinitely many) representative elements, e.g. those in an orthonormal basis, of their state spaces. Also, a linear algebraic structure always resides in the state space of a quantum system. So, an algorithm checking a quantum system should be carefully developed so that the linear algebraic structure will not be broken.

II. Early Research on Model Checking of Quantum Systems

Despite the difficulties discussed in the previous section, quite a few model-checking techniques for quantum systems have been developed in the last 10 years. The earliest work mainly targeted checking quantum communication protocols:

- Taking the probabilism arising from quantum measurements into account, [23] used the probabilistic model-checker PRISM [34] to verify the correctness of quantum protocols, including superdense coding, quantum teleportation and quantum error correction.
- A branching-time temporal extension (called quantum computation tree logic or QCTL for short) of exogenous quantum propositional logic [37] was introduced and then the model-checking problem for this logic was studied in [5], [6], with verification of the correctness of quantum key distribution BB84 [8] as an application.
- A linear temporal extension QLTL of exogenous quantum propositional logic [37] was then defined and the corresponding model-checking problem was investigated in [38].
- Model-checking techniques were developed in [14], [15] for quantum communication protocols modelled in process algebra CQP (Communicating Quantum Processes) [22]. The checked properties are specified by the quantum computation tree logic QCTL defined in [6].
- A model-checker for quantum communication protocols was also developed in [24], [41], [25], where the checked properties are specified by QCTL [6] too, but only the protocols that can be modelled as quantum circuits expressible in the stabiliser formalism [26] were considered. In [21], [3], this technique was extended beyond stabiliser states and used to check equivalence of quantum protocols.

III. Model Checking Quantum Automata

A research line pursued by the authors and their collaborators is to develop model-checking techniques that can be used not only for quantum communication protocols but also for general quantum systems, including physical systems and quantum programs.

Quantum automata were adopted in [45], [35] as the model of the systems:

**Definition 3.1 (Quantum automata [33], [39])**: A quantum automaton is a 4-tuple \( A = (\mathcal{H}, \text{Act}, \{ U_\alpha : \alpha \in \text{Act} \}, \mathcal{H}_0) \), where:

1. \( \mathcal{H} \) is a finite-dimensional Hilbert space, called the state space;
2. \( \text{Act} \) is a finite set of action names;
3. for each action name \( \alpha \in \text{Act} \), \( U_\alpha \) is a unitary operator on \( \mathcal{H} \);
4. \( \mathcal{H}_0 \subseteq \mathcal{H} \) is the subspace of initial states.

A quantum automaton behaves as follows: it starts from some initial state in \( \mathcal{H}_0 \), and at each step it performs a unitary transformation \( U_\alpha \) for some \( \alpha \in \text{Act} \). An algorithm for checking certain linear-time properties (e.g. invariants and safety properties) was proposed in [45], where the corresponding model-checking problem was studied in [35].

IV. Model Checking Quantum Markov Chains

The model-checking problem for a larger class of quantum systems than quantum automata, namely quantum Markov chains and quantum Markov decision processes was studied in a series of papers by the authors and their collaborators [50], [48], [49], [28].

Continuous-time quantum Markov processes have been intensively studied in mathematical physics, and discrete-time quantum Markov chains were introduced in [47] as a semantic model for the purpose of termination analysis of quantum programs.

**Definition 4.1 (Quantum Markov chains [47])**: A quantum Markov chain is a triple \( (\mathcal{H}, \mathcal{E}, \mathcal{H}_0) \), where \( \mathcal{H} \) and \( \mathcal{H}_0 \) are the same as in Definition 3.1 and \( \mathcal{E} \) is a super-operator on \( \mathcal{H} \).

A quantum Markov chain starts in an initial state in \( \mathcal{H}_0 \), and at each step it performs (the same) quantum operation modelled by the super-operator \( \mathcal{E} \). Note that the (discrete-time) dynamics of closed quantum systems are usually depicted by unitary operators, and the behaviours of open quantum systems are described by super-operators (see [40], Section 8.2). Obviously, the notion of quantum automata can be generalised by replacing unitary operators \( U_\alpha \) in Definition 3.1 by super-operators \( \mathcal{E}_\alpha \) (\( \alpha \in \text{Act} \)). Furthermore, quantum Markov
Several algorithms for checking reachability of quantum Markov chains and quantum Markov decision processes were developed in [48], [49]. As in checking classical Markov chains and Markov decision processes, graph reachability is a key to these algorithms. However, classical graph theory is not suited to our purpose; instead a new theory of quantum graphs (i.e. graphs in a Hilbert space with adjacency relation induced by a super-operator) was developed, and in particular, an algorithm for the BSCC (bottom strongly connected components) decomposition of the state Hilbert spaces was found in [48]. Another decomposition technique, namely periodic decomposition, for quantum Markov chains was recently proposed in [28].

A labelled super-operator-valued Markov chain over a set $A P$ of predefined atomic propositions is a 5-tuple $(S, s_0, \mathcal{H}, Q, L)$, where:

1. $S$ is a finite set of classical states with $s_0 \in S$ being the initial state;
2. $\mathcal{H}$ is a finite-dimensional Hilbert space, called the quantum state space;
3. $Q : S \times S \rightarrow SO_\mathcal{H}$ is a transition super-operator function, where $SO_\mathcal{H}$ denotes the set of trace-nonincreasing super-operators on $\mathcal{H}$, and for each $s \in S$, $\sum_{t \in S} Q(s, t)$ is trace-preserving; and
4. $L : S \rightarrow 2^{AP}$ is a labelling function.

A super-operator-valued Markov chain has two state spaces, a classical one and a quantum one, which are connected through the transition super-operator function. It behaves in a similar manner as classical Markov chains. It starts from the classical initial state $s_0$ and with the quantum initial state unspecified (it can be taken arbitrarily). Then at each step, given the current classical state $s$ and quantum state $\rho$, it proceeds to classical state $t$ with probability $tr[Q(s, t)(\rho)]$, and the accompanied quantum state evolves into $Q(s, t)(\rho)/tr[Q(s, t)(\rho)]$ provided that $\sum_{t \in S} Q(s, t)(\rho) \neq 0$. The normalisation requirement that $\sum_{t \in S} Q(s, t)$ is trace-preserving guarantees that the probabilities of going from $s$ to some classical state sum up to 1.

As the atomic propositions are taken to be classical (they apply only to classical states), this Markov chain model is suitable for verification of quantum systems against classical properties, such as running time, termination, reachability, etc. One distinct feature of this model, however, for verification purpose, is that it provides a way to check once-for-all in that once a property is checked to hold, it holds for all initial quantum states. For example, for the reachability problem, the model checking algorithm essentially calculates a positive operator $\Pi$, accounting for all (classical) paths satisfying the concerned property. Then the reachability probability when the Markov chain is started in the initial quantum state $\rho$ is simply $tr(\Pi \rho)$.

A corresponding computation tree logic (CTL) for super-operator-valued Markov chains was defined, and algorithms for checking such properties were developed in [18]. A tool implementation of these algorithms has been provided [19] based on the probabilistic model checker ISCASMC [30]. Algorithms for model checking $\omega$-regular properties, a very general class of properties subsuming those expressible by LTL formulae, against super-operator-valued Markov chains were proposed in [20]. This allows to express and analyse a wide range of relevant properties, such as repeated reachability, reachability in a restricted order, nested Until properties, or conjunctions of such properties. Furthermore, the reachability problem of a recursive extension of super-operator-valued Markov chains was studied in [21], with the application of analysing quantum programs with procedure calls.

V. MODEL CHECKING SUPER-OPERATOR-VALUED MARKOV CHAINS

The notion of super-operator-valued Markov chain is introduced in [18] as a higher-level model of quantum programs and quantum cryptographic protocols. A similar notion was proposed in [29] for a different purpose.

Definition 5.1 (Super-operator-valued Markov chains [18]): A labelled super-operator-valued Markov chain over a set $AP$ of predefined atomic propositions is a 5-tuple $(S, s_0, \mathcal{H}, Q, L)$, where:

1) $S$ is a finite set of classical states with $s_0 \in S$ being the initial state;
2) $\mathcal{H}$ is a finite-dimensional Hilbert space, called the quantum state space;
3) $Q : S \times S \rightarrow SO_\mathcal{H}$ is a transition super-operator function, where $SO_\mathcal{H}$ denotes the set of trace-nonincreasing super-operators on $\mathcal{H}$, and for each $s \in S$, $\sum_{t \in S} Q(s, t)$ is trace-preserving; and
4) $L : S \rightarrow 2^{AP}$ is a labelling function.

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VI. CONCLUSION

As reviewed in previous sections, several theoretical frameworks and algorithms of quantum model-checking have been developed. But certainly, quantum model-checking is still at a very early stage of its development; in particular, its applications are only at the level of toy examples. We envisage that in the future, quantum model-checking techniques can be applied to the following areas:

1) Checking physical systems: Physicists already considered the algorithmic checking problem of certain properties of quantum systems, for example, quantum measurement occurrence [17] and reachability of quantum states [42]. Quantum model-checking can offer a systematic view of this line of research.

2) Verification of quantum circuits: Verification of circuits has been one of the major application areas of classical model-checking. But model-checking applied to verification of quantum circuits is an area to be systematically exploited.

3) Analysis and verification of quantum programs: Another important application area of classical model-checking is analysis and verification of programs. Several techniques for analysis and verification of quantum programs have been reported in the last few years [32], [43], [44], [46]. However, model-checking techniques specifically designed for quantum programs are still missing.

4) Verification of security of quantum communication protocols: Applications of model-checking mentioned in Section III focus on verification of correctness of quantum communication protocols. But verification of the security of quantum protocols is much more difficult, and model-checking applied to it is an interesting topic for future research.

Finally, a crucial step toward real-world applications of model-checking would be building efficient automatic tools.
