Model Checking Applied to Quantum Physics

Ji Guan[1,2], Yuan Feng[2], Andrea Turrini[1] and Mingsheng Ying[1,2,3]

[1] State Key Laboratory of Computer Science, Institute of Software, Chinese Academy of Sciences, Beijing 100190, China
[2] Center for Quantum Software and Information, University of Technology Sydney, NSW 2007, Australia
[3] Department of Computer Science and Technology, Tsinghua University, Beijing 100084, China

Abstract. Model checking has been successfully applied to verification of computer hardware and software, communication systems and even biological systems. In this paper, we further push the boundary of its applications and show that it can be adapted for applications in quantum physics. More explicitly, we show how quantum statistical and many-body systems can be modeled as quantum Markov chains, and some of their properties that interest physicists can be specified in linear-time temporal logics. Then we present an efficient algorithm to check these properties. A few case studies are given to demonstrate the use of our algorithm to actual quantum physical problems.

Full Version: ArXiv:1902.03218

Two Model Checking Problems from Quantum Physics— Our motivations are two problems from two different fields of quantum physics:

Quantum Statistical Mechanics: *Quantum statistical mechanics* is essentially statistical mechanics applied to quantum systems. It is based on the statistical description of measurements [11]. Specifically, through observing state ρ_t (Hermitian positive semidefinite matrix with unit trace) of a quantum system (a finite-dimensional Hilbert space) at time t with a *quantum measurement* (e.g., position and momentum), which is mathematically modeled by a set $\{M_k\}_{k=1}^m$ of matrices on $\mathcal{H}$ with $\sum_k M_k^\dagger M_k = I$ (the identity operator on $\mathcal{H}$), the probability of outcome k is $p_k = \mathrm{tr}(M_k^\dagger M_k \rho_t)$.

Quantum statistical mechanics is mainly concerned with the connections between the classical information (probability distributions of measurement outcomes) and the quantum information (quantum states) of quantum systems. A fundamental problem in the foundations of it is the long-term classical information of quantum systems. It originated from John von Neumann's 1929 paper on the quantum ergodic theorem [4, 10], which asserts that for an appropriate finite set of mutually commuting measurements, every initial quantum state evolves so that for most time in the long run, the joint probability distribution of these measurements is close to a certain distribution. A renewed interest in recent years leads to the study of long-term properties of the measurement outcome distribution $(\mathrm{tr}(M_1^\dagger M_1 \rho_t), \mathrm{tr}(M_2^\dagger M_2 \rho_t), \ldots, \mathrm{tr}(M_n^\dagger M_n \rho_t))$ [5, 8, 9]; especially,

*Problem 1 (**Long-term classical information**).* Let $\{\mathcal{I}_l\}_{l=1}^n$ be a finite set of intervals in $[0, 1]$ and $\{M_k\}_{k=1}^m$ a measurement. Given a multiset $\{l_k : 1 \le l_k \le n\}_{k=1}^m$, is $\mathrm{tr}(M_k^\dagger M_k \rho_t)$ eventually (respectively, infinitely often) in $\mathcal{I}_{l_k}$ for all $1 \le k \le m$?

Quantum Many-body Systems: A *quantum many-body system* is a complex system of multiple interacting microscopic particles [12]. The number of particles can be near or more than 10^{20} when we consider *thermodynamic limit* (of *quantum condensed matter*) in practice, and the dimension of the state space for the whole system (all particles) is at least $2^{10^{20}}$. *Quantum many-body problems* are concerned with bulk properties (e.g., superfluidity and superconductivity) of such large systems. Obviously, exact or analytical solutions to them are impractical or even impossible. A common approach is to find hypothetical models that capture some essential aspects (e.g., ground states and ground energy) of the real systems, such as *Matrix Product States (MPS)* and *Tensor Product States*

(TPS) in terms of the topological structure of the systems [12]. Let us consider an 1-dimensional MPS as an example. Assume the system consists of N quantum particles in a line, indexed from 1 to N, and each particle has its own d-dimensional Hilbert space, denoted by $\mathcal{H}_d$. Then the entire Hilbert space is $\mathcal{H} = \mathcal{H}_d^{\otimes N}$. MPSs have the form:

$$|\psi_N\rangle = \sum_{k_1,\dots,k_N=1}^{d} \mathrm{tr}(A_{k_1}\cdots A_{k_N})|k_1\rangle \otimes \cdots \otimes |k_N\rangle \tag{1}$$

where $\{|k\rangle\}_{k=1}^d$ is an orthonormal basis of $\mathcal{H}_d$ and $\{A_k\}_{k=1}^d$ is a family of $D \times D$ complex matrices with D being independent on N and describing the entanglement strength.

For verifying the validity of matrices $\{A_k\}$ in the hypothetical model (1) of an MPS in thermodynamic limit ($N \to \infty$), we need to answer:

*Problem 2 (**Dichotomy problem**).* Given a finite set of $D \times D$ complex matrices $\{A_k\}$ and a positive integer J. (1) Is $|\psi_N\rangle \neq 0$ for all $N \geq J$? (2) Is there $N_0 \geq J$ such that $|\psi_N\rangle \neq 0$ for all $N \geq N_0$?

Our Contributions— We develop an efficient model checking algorithm solving Problems 1 and 2. First, we show that quantum statistical and many-body systems can be modeled as *quantum Markov chains (QMCs)*. For the flexibility of applications, we admit *abstract* linear-time temporal logic (LTL) formulas, which can specify the properties in Problems 1 and 2. We further give an effective procedure to approximately answer the LTL model checking problem for QMCs. The main technique is based on the *eigenvalue-analysis* of QMCs, which significantly simplifies the previous work based on decompositions of the state space [1].

Quantum Markov Chains— QMCs are a straightforward generalization of classical Markov chains. A QMC is a tuple $\mathcal{G} = (\mathcal{H}, \mathcal{E}, \rho_0)$, where $\mathcal{H}$ is a Hilbert space, $\mathcal{E} \in \mathcal{S}(\mathcal{H})$ a super-operator (a completely positive and trace-preserving map) on $\mathcal{H}$, and $\rho_0 \in \mathcal{D}(\mathcal{H})$ an initial state. Here, $\mathcal{S}(\mathcal{H})$ and $\mathcal{D}(\mathcal{H})$ are the set of all super-operators and quantum states on $\mathcal{H}$, respectively. Especially, $\mathcal{G}$ is called *irreducible* if $\mathcal{E}$ has only one full-rank stationary state [3]; that is, there exists a unique $\rho \in \mathcal{D}(\mathcal{H})$ such that $\mathcal{E}(\rho) = \rho$, and further $\rho > 0$, i.e., ρ is strictly positive.

The state transitions of $\mathcal{G}$ can be described as the *trajectory*: $\sigma_s(\mathcal{G}) = \rho_0, \mathcal{E}(\rho_0), \mathcal{E}^2(\rho_0), \dots$. Sometimes, quantum states are not our concern in practice. Then a QMC can be defined as a pair $\mathcal{G} = (\mathcal{H}, \mathcal{E})$ without explicitly specifying the initial state, and its behavior described by the trajectory of super-operators: $\sigma_d(\mathcal{G}) = \mathrm{id}_{\mathcal{H}}, \mathcal{E}, \mathcal{E}^2, \dots$.

Linear-Time Properties in Quantum Physics—In this paper, we present two *linear-time temporal logics* (LTLs) as languages for specifying properties of quantum physical systems. Our logics are essentially the same as the ordinary LTL except that its atomic propositions are interpreted in quantum physics.

Atomic Propositions Interpreted in Quantum Statistics— A *physical observable* is modeled by a Hermitian operator A in the state Hilbert space $\mathcal{H}$, i.e., $A^\dagger = A$. Then a quantum measurement can be constructed from A as follows. An *eigenvector* of A is a non-zero vector $|\psi\rangle \in \mathcal{H}$ such that $A|\psi\rangle = \lambda|\psi\rangle$ for some complex number λ (indeed, λ must be real when A is Hermitian). In this case, λ is called an *eigenvalue* of A. For each eigenvalue λ, the set $\{|\psi\rangle : A|\psi\rangle = \lambda|\psi\rangle\}$ of eigenvectors corresponding to λ together with the zero vector is a subspace of $\mathcal{H}$. We write P_λ for the projection onto this subspace. Then we have the spectral decomposition [6, Theorem 2.1]: $A = \sum_\lambda \lambda P_\lambda$, where λ ranges over all eigenvalues of A. Moreover, $M = \{P_\lambda\}_\lambda$ is a (projective) measurement. If we perform M on the quantum system in state ρ, then the outcome λ is obtained with probability $p_\lambda = \mathrm{tr}(P_\lambda^\dagger P_\lambda \rho) = \mathrm{tr}(P_\lambda \rho)$, and the expectation of A in state ρ is $[\![A]\!]_\rho = \sum_\lambda p_\lambda \cdot \lambda = \sum_\lambda \lambda \mathrm{tr}(P_\lambda \rho) = \mathrm{tr}(A\rho)$. Our atomic propositions are chosen to give an estimation of the expectations of physical observables.

Definition 1. *1. An atomic proposition in a Hilbert space $\mathcal{H}$ is defined as a pair $(A, \mathcal{I})$, where A is an observable in $\mathcal{H}$ and $\mathcal{I} \subseteq \mathbb{R}$ is an interval.*
2. A state $\rho \in \mathcal{D}(\mathcal{H})$ satisfies $a := (A, \mathcal{I})$, written $\rho \models a$, if the expectation of A in ρ lies in interval $\mathcal{I}$: $\mathrm{tr}(A\rho) = [\![A]\!]_\rho \in \mathcal{I}$.

As usual, we assume a finite set AP of atomic propositions. Now let us extend the satisfaction relation $\rho \models a$ to $\mathcal{G} \models \varphi$ between a QMC $\mathcal{G}$ and a general LTL formula φ. To this end, we introduce the labeling function: $L_s \colon \mathcal{D}(\mathcal{H}) \to 2^{AP}, L_s(\rho) = \{\, a \in AP : \rho \models a \,\}$ which assigns to each quantum state the set of atomic propositions in AP satisfied by the state. We further extend the labeling function to sequences of quantum states by setting $L_s(\rho_0, \rho_1, \ldots) = L_s(\rho_0), L_s(\rho_1), \ldots$. Then we define: $\mathcal{G} \models_s \varphi$ if and only if $L_s(\sigma_s(\mathcal{G})) \in \mathcal{L}_\omega(\varphi)$, where $\mathcal{L}_\omega(\varphi) = \{\, \xi \in (2^{AP})^\omega : \xi \models \varphi \,\}$, the language containing all infinite words over 2^{AP} that satisfy φ.

Example 1. Given a quantum measurement $\{M_k\}_{k=1}^m$, we consider a sequence of physical observable $\{A_k = M_k^\dagger M_k\}_{k=1}^m$ and a finite set of intervals $\{\mathcal{I}_l\}_{l=1}^n$ in $[0,1]$. Let $AP = \{(A_k, \mathcal{I}_l) : 1 \le k \le m, 1 \le l \le n\}$ with atomic proposition $(A_k, \mathcal{I}_l)$ asserting that expectation $\mathrm{tr}(A_k \rho) \in \mathcal{I}_l$. Then Problem 1 can be rephrased as: Given a multiple set $\{l_k : 1 \le l_k \le n\}_{k=1}^m$, is $\mathcal{G} \models_s \bigwedge_{k=1}^m \Box(A_k, \mathcal{I}_{l_k})$ (respectively, $\mathcal{G} \models_s \bigwedge_{k=1}^m \Box\Diamond(A_k, \mathcal{I}_{l_k})$)?

Atomic Propositions Interpreted in Quantum Many-Body Systems— First, note that given $|\psi_N\rangle$ in Eq. (1), there exists an orthogonal decomposition $\mathcal{H}_D = \bigoplus_m \mathcal{H}_{D,m}$ such that $|\psi_N\rangle$ can be linearly represented by a set of families of operators $\{\{B_{m,j} \in \mathcal{B}(\mathcal{H}_{D,m})\}_j\}_m$, where $\mathcal{E}_m(\cdot) = \sum_j B_{m,j} \cdot B_{m,j}^\dagger$ is a super-operator and $(\mathcal{H}_{D,m}, \mathcal{E}_m)$ is irreducible, with positive coefficients $\{a_m > 0\}_m$: $|\psi_N\rangle = \sum_m a_m |\phi_{N,m}\rangle$, where $|\phi_{N,m}\rangle = \sum_{k_1,\ldots,k_N} \mathrm{tr}(B_{m,k_1} \cdots B_{m,k_N}) |k_1\rangle \cdots |k_N\rangle$. This representation is called the *irreducible form* in [2] and it can be effectively computed. Therefore, $|\psi_N\rangle = 0$ if and only if $|\phi_{N,m}\rangle = 0$ for all m. Without loss of generality, from now on, we always assume that the set $\{A_k\}$'s corresponds to an irreducible QMC $(\mathcal{H}_D, \mathcal{E})$ with $\mathcal{E}(\cdot) = \sum_k A_k \cdot A_k^\dagger$. Further, $|\psi_N\rangle = 0$ if and only if $\langle \psi_N | \psi_N \rangle = 0$. By simple calculations, we have $\langle \psi_N | \psi_N \rangle = \mathrm{tr}([\sum_k E_k^* \otimes E_k]^N) = \mathrm{tr}([M_\mathcal{E}^N]^*) = \mathrm{tr}(M_\mathcal{E}^N)$ where E^* stands for the (entry-wise) complex conjugate of E, $M_\mathcal{E} = \sum_k E_k \otimes E_k^*$ is called the *matrix representation* of $\mathcal{E}$, and the last equality in the above chain follows from $\mathrm{tr}(M_\mathcal{E})$ being a real number for any $\mathcal{E}$.

Definition 2. *1. An atomic proposition is defined to be an interval $\mathcal{I} \subseteq \mathbb{R}$.*
2. A super-operator $\mathcal{E} \in \mathcal{S}(\mathcal{H})$ satisfies $a := \mathcal{I}$, written $\mathcal{E} \models a$, if the trace of its matrix representation $M_\mathcal{E}$ lies in interval $\mathcal{I}$; that is, $\mathrm{tr}(M_\mathcal{E}) \in \mathcal{I}$.

The satisfaction relation $\mathcal{E} \models a$ can also be extended to $\mathcal{G} \models \varphi$ between a QMC $\mathcal{G}$ and an LTL formula φ. Here we use the labeling function: $L_d \colon \mathcal{S}(\mathcal{H}) \to 2^{AP}, L_d(\mathcal{E}) = \{\, a \in AP : \mathcal{E} \models a \,\}$ which assigns to each super-operator the set of atomic propositions in AP satisfied by it. Furthermore, let $L_d(\mathcal{E}_1, \mathcal{E}_2, \ldots) = L_d(\mathcal{E}_1), L_d(\mathcal{E}_2), \ldots$ for any sequence of super-operators $\mathcal{E}_1, \mathcal{E}_2, \ldots$. Therefore, we define: $\mathcal{G} \models_d \varphi$ if and only if $L_d(\sigma_d(\mathcal{G})) \in \mathcal{L}_\omega(\varphi)$.

Example 2. Given a finite set of matrices $\{A_k\}$ on a Hilbert space $\mathcal{H}$ corresponding to a (irreducible) QMC $\mathcal{G} = (\mathcal{H}, \mathcal{E})$ with $\mathcal{E}(\cdot) = \sum_k A_k \cdot A_k^\dagger$, we set $AP = \{\mathcal{I}_1, \mathcal{I}_2\}$, where $\mathcal{I}_1 = [0,0]$ and $\mathcal{I}_2 = (-\infty, 0) \cup (0, \infty)$. The atomic proposition $\mathcal{I}_1$ (resp. $\mathcal{I}_2$) asserts that the trace of the matrix representation of the current super-operator is zero (resp. nonzero). The properties considered in Problem 2 can be written as the LTL formulas: (1) Is $\mathcal{G} \models_d \bigcirc^{(J)} \Box \mathcal{I}_2$? (2) Is $\mathcal{G} \models_d \bigcirc^{(J)} \Diamond\Box \mathcal{I}_2$?

Model Checking Algorithm—In the end, we develop an effective algorithm to answer the LTL model checking problem for QMCs. In the meanwhile, we run experiments on AKLT (Affleck-Kennedy-Lieb-Tasaki) and cluster models, which are two essential 1-dimensional quantum many-body systems [7]. The results illustrate how our algorithm can be applied in quantum physics.

Theorem 1 (Informal). *Verifying $\mathcal{G} \models_s \varphi$ and $\mathcal{G} \models_d \varphi$ can be effectively and approximately answered.*

References

1. M. Agrawal, S. Akshay, B. Genest, and P. Thiagarajan. Approximate verification of the symbolic dynamics of markov chains. *Journal of the ACM (JACM)*, 62(1):2, 2015.
2. G. De las Cuevas, J. I. Cirac, N. Schuch, and D. Perez-Garcia. Irreducible forms of matrix product states: Theory and applications. *Journal of Mathematical Physics*, 58(12):121901, 2017.
3. F. Fagnola and R. Pellicer. Irreducible and periodic positive maps. *Communications on Stochastic Analysis*, 3(3):407–418, 2009.
4. S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghì. Long-time behavior of macroscopic quantum systems. *The European Physical Journal H*, 35(2):173–200, 2010.
5. N. Linden, S. Popescu, A. J. Short, and A. Winter. Quantum mechanical evolution towards thermal equilibrium. *Physical Review E*, 79(6):061103, 2009.
6. M. A. Nielsen and I. L. Chuang. *Quantum computation and quantum information*. Cambridge university press, 2010.
7. D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac. Matrix Product State Representation. *Quantum Inf. Comp.*, 7:401, 2007.
8. S. Popescu, A. J. Short, and A. Winter. Entanglement and the foundations of statistical mechanics. *Nature Physics*, 2(11):754, 2006.
9. M. Rigol, V. Dunjko, and M. Olshanii. Thermalization and its mechanism for generic isolated quantum systems. *Nature*, 452(7189):854, 2008.
10. J. von Neumann. Beweis des ergodensatzes und desh-theorems in der neuen mechanik. *Zeitschrift für Physik*, 57(1-2):30–70, 1929.
11. J. von Neumann. *Mathematical Foundations of Quantum Mechanics: New Edition*. Princeton university press, 2018.
12. B. Zeng, X. Chen, D.-L. Zhou, and X.-G. Wen. Quantum information meets quantum matter. *arXiv preprint arXiv:1508.02595*, 2015.