Categorical Semantics for Schrödinger's Equation

Stefano Gogioso
Quantum Group
University of Oxford
stefano.gogioso@cs.ox.ac.uk

Applying ideas from monadic dynamics to the well-established framework of categorical quantum mechanics, we provide a novel toolbox for the simulation of finite-dimensional quantum dynamics. We use strongly complementary structures to give a graphical characterisation of quantum clocks, their action on systems and the relevant energy observables, and we proceed to formalise the connection between unitary dynamics and projection-valued spectra. We identify the Weyl canonical commutation relations in the axioms of strong complementarity, and conclude the existence of a dual pair of time/energy observables for finite-dimensional quantum clocks, with the relevant uncertainty principle given by mutual unbias of the corresponding orthonormal bases. We show that Schrödinger's equation can be abstractly formulated as characterising the Fourier transforms of certain Eilenberg-Moore morphisms from a quantum clock to a quantum dynamical system, and we use this to obtain a generalised version of the Feynman's clock construction. We tackle the issue of synchronism of clocks and systems, prove conservation of total energy and give conditions for the existence of an internal time observable for a quantum dynamical system. Finally, we identify our treatment as part of a more general theory of simulated symmetries of quantum systems (of which our clock actions are a special case) and their conservation laws (of which energy is a special case). This is a summary of [10]. The technical details on representation theory in Categorical Quantum Mechanics, used throughout this work, are collected in the companion paper [12].

1 Background

The Categorical Quantum Mechanics (CQM) programme [1] [13] [2] [4] is concerned with the understanding, through the language of category theory, of the structural and operational features of quantum theory. The sequential and parallel aspects of quantum processes are captured by the compositional and symmetric monoidal structures of the category fdHilb of finite-dimensional Hilbert spaces and linear maps. State/operator duality, corresponding to the Shrödinger/Heisemberg picture duality in quantum dynamics, finds its categorical formulation in the †-compact structure of fdHilb.

The investigation of classical-quantum duality goes through the definition of classical structures [5] [6], i.e. special commutative †-Frobenius algebras. Shown to correspond to orthonormal bases in fdHilb, classical structures are key to the operational characterisation of quantum measurements, controlled operations and completely positive maps. Interaction between different classical structures can be understood by introducing requirements of coherence, complementarity (a.k.a. Hopf law) and strong complementarity (a.k.a. bialgebra equations): strongly complementary structures play a fundamental role in the formulation of non-locality [3], and are exactly classified by finite abelian groups [14].

The categorical approach to theories of physical systems and transformations is perhaps best argued in [7] and the collected works [13] [2], and it provides the starting point for the formulation of the *monadic dynamics* framework [11]. In the same spirit of physical simulation as [8] [9], the framework aims at a categorical formulation of the operational aspects of dynamics, internalising notions of time via simulation by physical systems (a.k.a. clocks); dynamical systems are identified as the objects of the Eilenberg-Moore category for a certain monad encoding the dynamical structure of the clock.

Submitted to:
QPL 2015

In the context of quantum theory, this idea yields a quantum clock similar to that presented in [8], with complex unitary representations of finite groups giving the quantum dynamical systems. Furthermore, monadic dynamics can be used to model quantum circuits, and yield the Feynman's clock construction as a corollary: the construction, originally introduced in [8] and recently revisited in [15], plays a central role in simulated quantum dynamics, as it provides a way of computing whole histories of states in quantum circuits by finding the ground states of a certain Hamiltonian.

2 Summary of the work

Categorical Quantum Mechanics aspires to be the formalism of choice for the description of quantum algorithms (see, for example, the work in [16]), but currently lacks adequate tools for the description of the dynamical aspects of quantum mechanics. The main aim of this paper is to cover this gap, opening the way for a systematic application of the framework to the field of simulated quantum dynamics.

We introduce quantum clocks in the CQM formalism, encoding their time translation group in a strongly complementary pair of classical structures, and proceed to define quantum dynamical systems governed (or simulated) by them, in the form of Eilenberg-Moore algebras. We identify the classical structures of the strongly complementary pair as the non-degenerate observables for the time states and the energy levels of the clock. Using the duality between unitary dynamics and observables, we define Hamiltonians (which are coalgebraic objects) as the adjoints of unitary dynamics (which are algebraic objects). We provide the Fourier transform and prove that the eigenvalues of the Hamiltonians find their natural environment in the Pontryagin dual of the time translation group (its group of multiplicative characters). We give the proof of Von Neumann's mean ergodic theorem within the framework, identifying time-averages for the evolution of a quantum dynamical system with ground states of the Hamiltonian.

We prove that strong complementarity is the same as canonical commutation, in the sense of the Weyl CCRs, and we conclude that clocks necessarily possess a conjugate pair of time/energy observables. Using demolition measurements, we prove the time/energy uncertainty principle as a consequence of complementarity. We give a categorical definition of Schrödinger's equation as the energy perspective on the defining equation for Eilenberg-Moore morphisms. We identify quantum circuits as certain composite quantum dynamical systems, define stationary flows of states through them and prove the validity of the Feynman's clock construction within our framework.

We define synchronisation of quantum clocks with quantum dynamical systems (the "real world" counterpart for the quantum dynamics defined in this work), and show how "forgetting" a clock induces a conserved total energy for the remaining synchronised systems. We define internal time observables and give necessary and sufficient conditions for their existence. We also give conditions under which a system in a synchronised family can be turned into a clock governing all the other systems.

Finally, we prove a finite-dimensional analogue to Stone's Theorem on 1-parameter unitary groups (the result traditionally linking continuous-time dynamics to Hamiltonians and energy) that applies to our case. We briefly revisit this work in the light of a more general theory of symmetries of quantum systems, and explain how such a generalisation could be achieved in the framework of CQM.

Acknowledgements

The author would like to thank Bob Coecke, Aleks Kissinger, Clare Horsman, Amar Hadzihasanovic, Will Zeng, Sukrita Chatterji and Nicolò Chiappori for plenty of comments, suggestions, useful discussions and support. Funding from EPSRC and Trinity College is gratefully acknowledged.

References

[1] S. Abramsky & B. Coecke: *Categorical Quantum Mechanics*. doi:10.1016/B978-0-444-52869-8.50010-4. Available at `http://arxiv.org/abs/0808.1023`.

[2] B. Coecke, editor (2011): *New Structures for Physics*. Springer, doi:10.1007/978-3-642-12821-9.

[3] B. Coecke, R. Duncan, A. Kissinger & Q. Wang (2012): *Strong Complementarity and Non-locality in Categorical Quantum Mechanics*. Available at `http://arxiv.org/abs/1203.4988v2`.

[4] B. Coecke & A. Kissinger (2015 (to appear)): *Picturing Quantum Processes*. Cambridge University Press.

[5] B. Coecke, E. O. Paquette & D. Pavlovic: *Classical and quantum structuralism*. Available at `http://arxiv.org/abs/0904.1997`.

[6] B. Coecke & D. Pavlovic: *Quantum measurements without sums*. doi:10.1201/9781584889007.ch16. Available at `http://arxiv.org/abs/quant-ph/0608035`.

[7] A. Doering & C. J. Isham (2007): *A Topos Foundation for Theories of Physics: IV. Categories of systems*. Available at `http://arxiv.org/abs/quant-ph/0703066v1`.

[8] R. P. Feynman (1982): *Simulating physics with computers*. International Journal of Theoretical Physics, doi:10.1007/BF02650179.

[9] T. Fritz (2011): *Quantum graphenity*. Available at `http://fqxi.org/data/essay-contest-files/Fritz_essay.pdf`.

[10] S. Gogioso (2015): *Categorical Semantics for Schrodinger's Equation*. Available at `http://arxiv.org/abs/1501.06489`.

[11] S. Gogioso (2015): *Monadic dynamics*. Available at `http://arxiv.org/abs/1501.04921`.

[12] S. Gogioso & W. Zeng (2015): *Fourier transforms from strongly complementary observables*. Available at `http://arxiv.org/abs/1501.04995`.

[13] H. Halvorson, editor (2011): *Deep Beauty*. Cambridge University Press, doi:10.1017/CBO9780511976971.

[14] A. Kissinger (2012): *Pictures of Processes: Automated Graph Rewriting for Monoidal Categories and Applications to Quantum Computing*. Ph.D. thesis. Available at `http://arxiv.org/abs/1203.0202`.

[15] J. R. McClean, J. A. Parkhill & A. Aspuru-Guzik (2013): *Feynman's clock, a new variational principle, and parallel-in-time quantum dynamics*. Available at `http://arxiv.org/abs/1301.2326`.

[16] J. Vicary (2013): *The Topology of Quantum Algorithms*. *LICS*, doi:10.1109/LICS.2013.14. Available at `http://arxiv.org/abs/1209.3917`.