PROJECT DESCRIPTION

QUANTUM TECHNIQUES FOR STOCHASTIC PHYSICS

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1. Introduction

Techniques from quantum field theory can also be applied to collections of randomly interacting *classical* particles. This surprising fact has already been noted by many authors, starting perhaps with Doi [9] in 1976. This fact is, however, just the tip of a deeper iceberg. One can take quantum theory, systematically replace amplitudes by probabilities, and obtain a collection of new techniques for studying 'stochastic physics': that is, the physics of classical systems with random interactions.

Examples arise in a host of different fields. Chemists often describe chemical reactions in a stochastic rather than quantum-mechanical way using the formalism of 'chemical reaction networks' [10, 16]. Computer scientists study random processes using an equivalent formalism: 'stochastic Petri nets' [17, 18]. Many important models in population biology [8, 19] and biochemistry [14, 15] are also described by these formalisms. While these formalisms are *secretly* a way of writing down models of stochastic physics in terms of creation and annihilation operators, this fact is unknown to most people using them.

Work on models formulate this way has been carried out by diverse communities of researchers including chemists, computer scientists and biologists. Unfortunately, these communities have not always communicated their results among each other. Many have also failed to note that the underlying mathematics has been deeply studied within mathematical physics. Conversely, most mathematical physicists are unaware of the large body of relevant work in these other disciplines.

During a recent 2-year visit to the Centre for Quantum Technologies, the PI began to address these problems. The first step was to write a textbook with the help of Jacob Biamonte, entitled *A Course on Quantum Techniques for Stochastic Mechanics*. Freely available on the arXiv in draft form [5], this book explains how techniques from quantum physics can be extended to stochastic physics. Not merely a summary of existing work, it also brings more tools from quantum theory—for example Noether's theorem [6] and coherent states—to bear on stochastic many-body processes. It contains a rich set of examples taken from chemistry, biology and other subjects.

Building on this foundation, the project funded by this grant will develop quantum techniques for stochastic physics still further, with the help of two graduate students and two expert visitors, and publicize the results to a large audience. More specifically, the project will do the following five things:

1. Study the approach to equilibrium. Mathematically minded chemists have already proved a number of powerful theorems on equilibrium states, and the approach to equilibrium, for stochastic many-body processes [1, 10, 16]. However, quantum techniques will give significant improvements of their work. This is especially true when 'finite size effects' are important: in other words, when we cannot take the limit as the number of interacting objects involved goes to infinity, this being analogous to a 'classical limit'.

2. Study stochastic systems with more complex behavior. Systems that fail to converge to a unique equilibrium are also important, especially in biology. Systems that exhibit periodic behavior can function as 'biological clocks' [13], while systems with more than one stable state can function as 'switches' in living organisms [7, 12]. Besides studying systems with simple equilibrium behavior, the research funded by this grant will also use quantum techniques to study these more complex and interesting phenomena.

3. Train students working at the interface of quantum and stochastic physics. This grant will mainly go to provide salary support for two Graduate Student Researchers for 6 academic months per year at 49% for three years. It will also fund these students to attend conferences. These students will help with the projects described above, and go on to do their theses on quantum techniques for stochastic physics. The PI currently has five graduate students who want to begin work with him. Of these, two have done undergraduate work in physics (Franciscus Rebro and Blake Pollard) while one has already published on stochastic processes (Michael Knap). The PI will use this grant to fund the two students who are best suited to the project.

4. Initiate collaboration between mathematical physicists and mathematical chemists. The grant will also pay for two experts in mathematical chemistry to visit U. C. Riverside. Candidates include Anne Shiu of the Department of Mathematics at the University of Chicago and Gavin Crooks of Physical Biosciences Division at Lawrence Berkeley National Laboratory. Shiu is deeply involved in chemical reaction networks, while Crooks is an expert on the physics of stochastic processes.

5. Publicize the results obtained. The PI will publicize the results of this research and these visits using his blog and also in a book and lectures. His blog, *Azimuth*, is widely read, and has attracted an audience of scientists interested in quantum techniques for stochastic processes [2]. Indeed, the PI wrote a draft of his book *A Course on Quantum Techniques for Stochastic Mechanics* with Jacob Biamonte 'on the blog', profiting greatly from interaction with the mathematicians, physicists and chemists following this course [4]. The PI will complete this book using the results obtained in the work funded by this grant. He is also a widely sought-after speaker, and has already given talks on this material in Singapore, Australia, Paris and Barcelona, together with a lecture course in Malaysia [3]. He will continue to give lectures on this topic, and especially on the new results obtained thanks to this grant.

2. Intellectual Merit and Broader Impacts

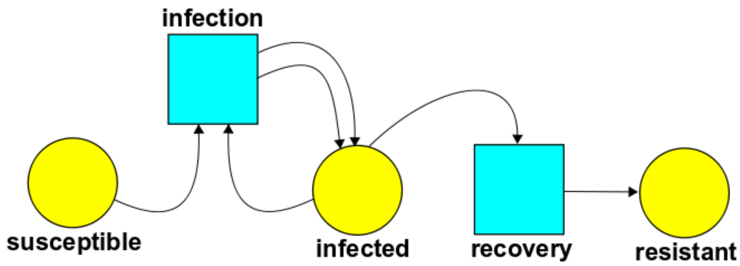
The **intellectual merit of the proposed activity** is that it will turn techniques from quantum physics toward a large new range of practical applications. These tools are often seen as being only applicable to quantum physics, not the macroscopic world we see around us. In fact, they are useful in stochastic physics as well, with potentially major benefits to chemistry, biology and other fields.

The **broader impacts resulting from the proposed activity** include starting a new dialogue between mathematical chemists and quantum field theorists, training graduate students versed in both subjects, and publicizing the use of quantum techniques to study stochastic physics, not only in a book and lectures, but also in the PI's blog.

3. Details

Quantum theory is based, not on probabilities, but on amplitudes. Of course can use amplitudes to compute probabilities. However, the relation between them is nonlinear: we take the absolute value of an amplitude and square it to get a probability. It thus seems very odd to treat amplitudes as *directly* analogous to probabilities. Nonetheless, if we do this, some good things happen. In particular, we can take techniques devised in quantum theory and apply them to probability theory. This sheds new light on old problems.

One of the basic objects of study in stochastic physics is a 'stochastic Petri net'. A stochastic Petri net describes in a very general way how collections of things of different kinds can randomly interact and turn into other things. Here is an example:



This is a simple model of an infectious diseases called the 'SIR model'. There are three 'states': **susceptible**, **infected** and **resistant**, shown as yellow circles. And there are two 'transitions': **infection**, where an infected person meets a susceptible person and infects them, and **recovery**, where an infected person recovers and becomes resistant to the diseases. There are also positive numbers called 'rate constants', not shown here, one for each transition.

Starting from any stochastic Petri net we can write down an equation called the 'master equation' which describes how the probability of having various numbers of things in each state changes with time. This takes the general form

$$\frac{d\Psi}{dt} = H\Psi$$

where the state Ψ describes the probability of having any given number of things in each state, and H is a linear operator, the 'Hamiltonian'.

A key realization is that this Hamiltonian can be written in terms of creation and annihilation operators, just as the Hamiltonians in quantum field theory. Surprisingly, the usual commutation relations for these operators hold, *even though we are discussing macroscopic objects not obeying Bose–Einstein statistics*. As a result, many of the usual ideas in quantum field theory can be adapted to this context. Of course, we must allow for the fact that Ψ describes probabilities rather than amplitudes. Thus the time evolution operators $\exp(tH)$ are not unitary; instead, they form a Markov semigroup. So, instead of H being self-adjoint, it must obey another condition: it must be 'infinitesimal stochastic'.

In the limit of large numbers, the master equation simplifies and we obtain a differential equation describing the rate of change of the *expected* numbers of things of each kind: the 'rate equation'. Feinberg, Horn and Jackson [10, 16] proved a powerful result classifying equilibrium solutions for the rate equation for a large class of stochastic Petri nets: the 'deficiency zero theorem'. Later, Anderson, Craciun and Kurtz [1] enhanced this result by showing how to obtain equilibrium solutions for the master equation in this case. (All these results were stated, not in terms of stochastic Petri nets, but in terms of another formalism: 'chemical reaction networks'. However, these formalisms are mathematically equivalent.)

The PI's book with Jacob Biamonte [5] presented new proofs of the deficiency zero theorem and Anderson–Craciun–Kurtz theorem. For the deficiency zero theorem, the key was to relate the rate equation to a certain Markov process. This was surprising, because the rate equation is nonlinear, while the equation describing a Markov process is linear in the probabilities involved. Nonetheless, equilibrium solutions of the Markov process give equilibrium solutions of the rate equation when the deficiency zero condition holds. Furthermore, a key step of the proof uses a new version of Noether's theorem, familiar from quantum physics but recently generalized to stochastic physics by Brendan Fong and the PI [6]. This theorem relates conserved quantities for Markov processes to operators that commute with the Hamiltonian. The advantage of the new proof is that it suggests ideas that apply even when the deficiency zero condition fails to hold.

For the Anderson–Craciun–Kurtz theorem, a new proof was given by the PI and Brendan Fong, which makes very clear the conceptual importances of techniques from quantum physics. The key is to consider 'coherent states', that is, eigenvectors of the annihilation operators. Using this, and the formula for the Hamiltonian in terms of annihilation and creation operators, one can easily find coherent states obeying

$$H\Psi = 0$$

By the master equation, we immediately obtain

$$\frac{d}{dt}\Psi = 0$$

which says that these coherent states Ψ are equilibrium solutions of the master equation.

In short, a host of new techniques can be imported from quantum physics to stochastic physics: annihilation and creation operators, Feynman diagrams, Noether's theorem and coherent states. These have just begun to be exploited. While it is too soon to say what the best results obtained using these new tools will be, there are some promising lines of attack, and the PI and his graduate students will start by pursuing these.

First, the new techniques will be used to gain more information about equilibrium solutions and the approach to equilibrium. While the deficiency zero theorem provides detailed information on this subject for the *rate equation*, for *a certain class* of stochastic Petri nets, it should be possible to get results for a much broader class, not only for the rate equation but also for the master equation. Indeed, many more results are already known for the rate equation, starting with the 'deficiency one theorem' [10, 11]. However, the new techniques will organize and further extend these results.

Second, it will be shown that for many stochastic Petri nets, uniqueness of equilibrium solutions, and convergence of other solutions to equilibrium solutions, are better-behaved for the master equation than for the rate equation. In particular, this is true for systems with solutions of the rate equation displaying periodic behavior [13], as in a 'biological clock', and systems with more than one stable state [7, 12], which can serve as 'switches' in biochemistry. This means that the large number limit, in which the master equation reduces to the rate equation, is somewhat singular in these cases. This limit should be very interesting from both a mathematical and physical point of view. In particular, if one treats the master equation as analogous to Schrödinger's equation, the rate equation is mathematically a kind of a 'classical limit' of this equation. This means that quantum techniques will be especially useful when finite size effects become important, and the master equation differs significantly from the rate equation.

4. Prior NSF Support

The PI has won two prior NSF grants. The most recent and relevant is award number 0653646, entitled 'Feynman Diagrams and the Semantics of Quantum Computation', a grant for $149,938.00 awarded in July 2007 and ending July 2012. The work done there, which provided a general foundation for theories involving Feynman diagrams, will at some point become important to the current project.

Summary of results, including broader impacts. In 'Physics, Topology, Logic and Computation: A Rosetta Stone', the PI and his graduate student Mike Stay, supported by this grant, worked out and carefully explained how Feynman diagrams, string diagrams in topology, proofs in logic, and processes of computation could all be dealt with in a unified way using symmetric monoidal categories with duals. Stay, who now works at Google, is now becoming an expert on categorical semantics and its applications to computer science. He is running a category theory mailing list at Google and is completing his Ph.D. thesis, which describes a theory of compact closed bicategories with duals in which computations are 2-morphisms.

After Mike Stay took a job at Google, most of the grant money went to supporting another graduate student of the PI, Alexander Hoffnung. Together with Hoffnung and another graduate student, Christopher Walker, the PI found that spans of groupoids are able to do much of what we normally do with linear operators in quantum theory. This was a rather unexpected turn. It turned out one can use this to 'groupoidify' a large portion of the mathematics of quantum theory, shedding light on its combinatorial underpinnings. Alexander Hoffnung has gone on to postdoctoral positions first at the University of Ottawa and now Temple University, and is carrying on this line of work. Christopher Walker has a tenure-track position at Odessa College.

In further work with his graduate students Christopher Rogers and John Huerta, the PI also studied the algebra of grand unified theories and applications of higher category theory to string theory. Thiese students have completed Ph.D.'s on closely related topics, and Christopher Rogers now has a postdoctoral position at the University of Göttingen, while John Huerta obtained postdocs first at Australian National University and now the Instituto Superior Técnico in Lisbon. Both are actively publishing more work along similar lines.

The PI gave several talks on the subject of the 'Rosetta Stone' paper. For example, he gave a one-hour plenary talk about it in 'Algebraic Topological Methods in Computer Science 2008' at University Paris 7 on July 7, 2008. The PI also gave a one-hour plenary talk at the '24th Annual IEEE Symposium on Logic in Computer Science' (LICS 2009) on August 13, 2009, and a colloquium talk at California State University, Fresno on April 9, 2010.

The PI also gave have also given talks on groupoidification. He spoke on this in October 2007 as the keynote speaker at 'Deep Beauty: Mathematical Innovation and the Search for an Underlying Intelligibility of the Quantum World', a workshop in honor of John von Neumann at Princeton University.The PI also spoke about it at the 'Groupoids in Analysis and Geometry' seminar in Berkeley on Tuesday May 20, 2008, at the conference 'Homotopy Theory and Higher Categories' at the Centre de Recerca Matemàtica (CRM) in Barcelona on June 30, and at the 2009 Joint Mathematics Meetings, Washington, D.C. in January 2009. The PI's students have also given many talks on the subjects of this research project.

Publications. The publications arising from grant number 0653646 were:

(1) J. Baez and A. Lauda, A prehistory of n-categorical physics, in *Deep Beauty: Mathematical Innovation and the Search for an Underlying Intelligibility of the Quantum World*, ed. Hans Halvorson, Cambridge U. Press, Cambridge, pp. 13–128.
(2) J. Baez, A. Hoffnung and C. Rogers, Categorified symplectic geometry and the classical string, *Comm. Math. Phys.* **293** (2010), 701–715.
(3) J. Baez and C. Rogers, Categorified symplectic geometry and the string Lie 2-algebra, *Homotopy, Homology and Applications* **12** (2010), 221–236.
(4) J. Baez, A. Hoffnung and C. Walker, Higher-dimensional algebra VII: groupoidification, *Th. Appl. Cat.* **24** (2010), 489–553.
(5) J. Baez and J. Huerta, The algebra of grand unified theories, *Bull. Amer. Math. Soc.* **47** (2010), 483–552.
(6) J. Baez and M. Stay, Physics, topology, logic and computation: a Rosetta Stone, in *New Structures for Physics*, ed. Bob Coecke, Lecture Notes in Physics vol. 813, Springer, Berlin, 2011, pp. 95–174.

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