Baez, John C.
Quantum techniques for reaction networks. (English) Zbl 1405.81184
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In chemistry, reaction networks are used to describe how various kinds of classical particles can interact to turn into other kinds. By way of examaple, the following reaction network gives a simplified picture of what is happening in a glass of water

$$H_2O \leftrightarrows H^+ + OH^-$$
$$H_2O + H^+ \leftrightarrows H_3O^+.$$

This paper aims at explaining how techniques from quantum mechanics, particularly second quantization, can be exploited to study reaction networks, which is a part of a broader program in investigation of links between quantum mechanics and stochastic mechanics, with probabilities replacing amplitudes ([the author and *B. Fong*, J. Complex Netw. 3, No. 1, 22–34 (2015; Zbl 1397.92783); J. Math. Phys. 54, No. 1, 013301, 8 p. (2013; Zbl 1280.81015); *J. C. Baez* and *J. D. Biamonte*, Quantum techniques in stochastic mechanics. Hackensack, NJ: World Scientific (2018; Zbl 1405.81005)]. Using second quantization methods to model classical stochastic systems can be traced back at latest to *M. Doi* ["Second quantization representation for classical many-particle system", J. Phys. A, Math. Gen. 9, No. 9, 1465–1477 (1976; doi:10.1088/0305-4470/9/9/008)], which has been further developed by *P. Grassberger* and *M. Scheunert* ["Fock-space methods for identical classical objects", Fortschritte Phys. 28, No. 10, 547–578 (1980; doi:10.1002/prop.19800281004)] and many others. Doi realized that spaces of generating functions are analogous to the Fock spaces in quantum theory and, in particular, that products of creation and annihilation operators can be used to depict stochastic processes where objects interact and turn into other objects. There is a long history in chemistry of sharp contrast between stochastic depiction of reactions by the master equation on the one hand and deterministic one by the rate equation on the other hand [*F. Horn* and *R. Jackson*, "General mass action kinetics", Arch. Ration. Mech. Anal. 47, No. 2, 81–116, (1972; doi:10.1007/BF00251225)].

The author argues how the master equation reduces to the rate equation in the large-number limit, just as a quantum field theory reduces to a classical field theory in the classical limit. The first towering theorem (Theorem 8) starts with the master equation, from which an equation for the rate of change of the expected number of particles of each species is derived. It is shown that the equation reduces to the rate equation in a certain approximation. The second towering theorem (Theorem 9) shows that the derived equation is no other than the rate equation in case that the numbers of particles of each species are described by independent Poisson distribution, relying on the benedictory fact that the generating function of a product of independent Poisson distributions is an eigenvector of all the annihilation operators. As is well known, many facts about classical mechanics are of simple generalizations to quantum mechanics as far as coherent states (i.e., eigenvectors of annihilation operators) [*J. R. Klauder* (ed.) and *B.-S. Skagerstam* (ed.), Coherent states. Applications in physics and mathematical physics. Singapore: World Scientific (1985; Zbl 1050.81558)]. The reader sees a similar phenomenon in stochastic mechanics, realizing that the deterministic dynamics governed by the rate equation matches the stochastic dynamics controlled by the master equation in the special case of coherent states. This view is further explored in [the author and Fong, loc. cit.].

Reviewer: Hirokazu Nishimura (Tsukuba)

MSC:

81V55 Applications of quantum theory to molecular physics
81T10 Model quantum field theories
81S22 Open systems, reduced dynamics, master equations, decoherence (quantum theory)
81Q20 Semi-classical techniques in quantum theory, including WKB and Maslov methods
82B30 Statistical thermodynamics
82B31 Stochastic methods in equilibrium statistical mechanics

Full Text: DOI

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