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Comment on mr-2021-50

Arthur Palmer (Referee)

Referee comment on "The Lindbladian form and the reincarnation of Felix Bloch's generalized theory of relaxation" by Thomas M. Barbara, Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-50-RC2, 2021

Paul Hubbard was a student with Edward Purcell at Harvard and then spent 40 years as a faculty member at the University of North Carolina at Chapel Hill. He passed away on October 30, 2020. The Raleigh News and Observer acknowledged in an obituary for Prof. Hubbard, "his research into nuclear magnetic resonance, the foundation of magnetic resonance imaging, and teaching mathematical methods of physics to generations of students". I was one of those students. Long before I was an NMR spectroscopist, and completely unaware of Prof. Hubbard's contributions, I was a graduate student in his course on Electricity and Magnetism in 1986. Only later as a postdoctoral fellow did I realize that the author of seminal papers on the theory of spin relaxation was my former instructor! The deep insight emerging from careful mathematical analysis evident in his papers also was a central aspect of his teaching.

In the present paper, Barbara reconsiders the contributions of Hubbard in the 1961 paper "Quantum-Mechanical and Semiclassical Forms of the Density Operator Theory of Relaxation" (Rev. Mod. Phys. 33 (1961) 249-264), and of parallel work by Bloch. Hubbard derives a quantum mechanical master equation for a spin system coupled to the surroundings. Barbara demonstrates that Hubbard's master equation is consistent with the LIndblad master equation for open quantum systems derived 15 years later. Hubbard himself does not seem to suggest applications of his theoretical results to problems outside of nuclear spin relaxation, but this might have been a consequence of the times: the laser had just been invented in 1960 and coherent optical spectroscopy lay in the future.

The Lindblad formalism was developed in 1976 in two papers and provides a general Markovian master equation for evolution of the density matrix. Lindblad, in "On the generators of quantum dynamical semigroups". Commun. Math. Phys. 48:119 (1976) does not appear to reference the field of NMR spin relaxation. Gorini et al. in "Completely positive dynamical semigroups of N-level systems". (J. Math. Phys. 17: 821(1976)) reference Bloch and Wangsness (Phys. Rev. 89:728 (1953)) and Abragam's "The Principles of Nuclear Magnetism", but neither Hubbard (1961) nor Bloch (Phys. Rev.

102:104 (1957)). Thus, the Lindbladian theory appears to have been developed independently of the related efforts in NMR spin relaxation, as noted by Barbara.

Barbara draws out the relationship between Hubbard's (and by extension, Bloch's) work in spin relaxation and the later work in open quantum systems by Lindblad and Gorini et al. The paper is very clearly written, but like Barbara, I recommend "A short introduction to the Lindblad master equation" (Manzano, AIP Advances 10.025106 (2020)) as a cogent introduction to Lindbladian formalism before reading the present paper. A very minor tyopgraphical error is that Manzano refers to the "rotating wave approximation", not the "rotating frame approximation" (line 306). Otherwise I did not find typographical errors beyond those already noted by other reviewers.

Lest the work by Barbara appear solely historical, Bengs and Levitt in "A master equation for spin systems far from equilibrium" (J. Magn. Reson. 310,106645 (2020)) recently introduced the Lindblad theory of open quantum systems into NMR spectroscopy to properly treat systems for which the assumptions of semi-classical Redfield theory do not hold. As described by Bengs and Levitt, modern NMR techniques, such as various hyper polarization methods, can generate states of the spin system outside the range of applicability of semi-classical relaxation theory. Thus, the linkages explored in the present paper by Barbara will be increasingly important to on-going developments in magnetic resonance.