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Comment on mr-2021-62

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Community comment on "Spin relaxation: is there anything new under the Sun?" by Bogdan A. Rodin and Daniel Abergel, Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2021-62-CC2>, 2021

In this submission Rodin and Abergel comment extensively on the 2020 paper by Christian Bengs and myself entitled "A master equation for spin systems far from equilibrium" (doi.org/10.1016/j.jmr.2019.106645). From the wording used by Rodin and Abergel, many readers will assume that (1) we stated in our paper that the "founding fathers" (Bloch, Redfield, Abragam) got the relaxation theory wrong, and (2) we introduced a new theory based on the Lindbladian equations that give the correct result. If Rodin and Abergel deliberately intended that impression to be conveyed, they would be guilty of a bad misrepresentation of our work. In fact, in our paper we state explicitly, many times, that the "founding fathers" were well aware, and mentioned explicitly many times over, the limitations of the semi-classical relaxation theory to a well-defined regime; and (2) the "founding fathers" were well aware that the crude "fix" that leads to the inhomogeneous master equation is invalid outside the assumptions of weak spin order and high spin temperature. In our paper we even cite extensively Redfield's phrase "unless the system is prepared in an unusual way". So if Rodin and Abergel mean to imply that we had stated that the "founding fathers" were unaware of the limitations of semi-classical relaxation theory, they are misrepresenting our work badly, and that impression should be corrected. The wording used by Rodin and Abergel is not entirely clear, so it is not obvious whether that accusation is their intention. Hopefully not. In any case, any possibility of a misrepresentation of our work should be corrected.

In our work we showed that the techniques of open quantum systems theory, and in particular the use of Lindbladian dissipation superoperators, may be used to formulate a relaxation equation which works outside the weak-order limit, bringing magnetic resonance into alignment with many other forms of spectroscopy. Within their paper, Rodin and Abergel appear to suggest a possibly different way to do this (it is not clear to me whether they propose that the result is different). They are certainly free to propose that, but it is unclear what the advantages would be over the existing and well-understood and widely used Lindbladian method.

Since our paper was published, Tom Barbara showed that the difficult exposition by Bloch and Hubbard leads to Lindbladian-like equations, many years before Lindblad. It is very possible that the "founding fathers" of magnetic resonance "pre-discovered" this key result of open quantum systems theorists. That is a fascinating analysis of the historical

development of magnetic resonance, but does not affect the conclusions we drew in our paper, or the way we represented the work of these giants. Incidentally, if Tom's analysis is correct (which is not in doubt), then Abragam seems to have missed this interesting path in his classic book. On pages 287-289, Abragam tries hard to find a formulation of relaxation theory which escapes the weak order approximation, but (in a rare weak passage) his exposition leads nowhere useful. Maybe the Bloch and Hubbard papers were too obscure, even for Abragam.

In summary, the new submission by Rodin and Abergel is a valuable contribution to the debate, but I hope they can pay more attention to the way they refer to our paper, and make sure that any way they represent our work is thoroughly validated and cannot be misread by a casual reader. To give a concrete example, they state in the abstract "..the underlying theory .. has been recently questioned" [by us]. This is not correct. We did not "question the underlying theory", in any way. On the contrary. We proposed a way to +implement+ the underlying theory outside the weak-order limit, making it clear that the proposed method is not our invention, but is standard outside the NMR world. Furthermore, Tom Barbara showed that at least Bloch and Hubbard anticipated a similar method many years before Lindblad.