Reply on CC7
Malcolm Levitt

Community comment on "Spin relaxation: under the sun, anything new?" by Bogdan A. Rodin and Daniel Abergel, Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-62-CC9, 2021

Just an additional comment, providing a little personal historical context. Speaking for myself, I had thought (arrogantly I guess) that this topic was essentially solved with Jeener and then myself (with Lorenzo Di Bari) introducing thermalized relaxation superoperators and avoiding the inhomogeneous master equation with its ugly and highly suspicious rho_eq term. It was only when Christian Bengs applied this to the ortho/para conversion of endohedral water in H2O@C60 (doi.org/10.1103/PhysRevLett.120.266001) that we realised there was something fundamentally wrong. I took quite some convincing since I suspected that Christian had just made some sort of mistake (I know better, now). Christian took this opportunity to dig into the open quantum systems literature (which was already an interest of his) and managed, with some trouble, to convince me that the double-commutator form could never give a relaxation superoperator appropriate for this regime, even with a thermalized correction applied afterwards, and formulated a Lindbladian-based treatment that does address this regime correctly as well as being thoroughly in line with the theoretical developments outside NMR. (Indeed, as you say, Daniel, there is nothing "new under the sun"). I want to put on record here how much credit Christian is due for his insight and persistence, in the face of opposition from myself. We now know, through Tom’s work, that at least some of the Lindbladian approach was anticipated much earlier by Bloch and Hubbard, although those papers are really tough, and the significance escaped even Abragam, who apparently overlooked this work, making two failed attempts in his book to address the problem. Apart from its historical interest, I personally see no reason to go over this ground again, since the Lindbladian formulation by Christian appears to have all possible advantages and to be solidly grounded. Clearly some in the community disagree (for example, a hostile referee blocked publication of our paper in J Chem Phys, with its broad readership) so it’s very appropriate that the competing interpretations are made available in the open scientific literature, for all to judge.