

Magn. Reson. Discuss., referee comment RC1 https://doi.org/10.5194/mr-2021-26-RC1, 2021 © Author(s) 2021. This work is distributed under the Creative Commons Attribution 4.0 License.

Comment on mr-2021-26

Anonymous Referee #1

Referee comment on "Hyperpolarization and the physical boundary of Liouville space" by Malcolm H. Levitt and Christian Bengs, Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-26-RC1, 2021

I we take spin 1/2 and express density matrix in terms of pauli matrices then the coordinates lie inside a Bloch sphere. The paper studies how does this result generalize to higher spins.

The paper studies density operator of a spin ensemble. Valid density operator are confined to reigons of Liouville space which authors call physical region. It is shown the phyical region is bounded by multidimensional figures called simplexes. vertex of which corresponds to pure state. Examples are given for spins 1/2, 1, 3/2 and coupled spins 1/2. Von Neumann entropy is used as a criterion for hyper polarization. It is shown that inhomogeneous master equation for spin dynamics leads to non physical results in some cases, a problem that may be avoided by using Lindbladian master equation.

In line 58, the other three operators should be Q2 Q3 Q4

In line 75, it is not known what zero quantum parts mean