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Interactive comment on "Representation of population exchange at level anti-crossings" *by* Bogdan A. Rodin and Konstantin L. Ivanov

Anonymous Referee #1

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In this work, Bodin and Ivanov give a thorough description of the use of the level anti-crossing concept to analyse population exchange in NMR experiments. The basic physical principles are given, and several applications are analysed with this formalism. This article is particularly welcome, considering the number and the importance of recent studies that rely on the LAC description to design new experiments. It is well written, in a clear and pedagogical way. I recommend publication in Magnetic Resonance, optionnally after the following comments have been addressed.

Main comments:

The formalism described here is very powerful to identify the possibility of population exchange (existence of a LAC) and qualitatively what happens to the population. In the examples analysed here, no expression is given for the parameter Delta, as the

function of exprimental parameters, be it for the adiabatic or the non adiabatic transfers. In other words, Eq. 7 and 8 are not reused. Is the formalism moslty useful for qualitative analyses ?

The notion that a LC is "converted into a LAC" is sometimes confusing, especially when the conversion seems to be described as a dynamic process while the perturbation is an internal interaction of the spin system. Is that common QM jargon ? For example, on l. 302 "which are never converted into a LAC" is confusing, since nothing can change anyway. Perhaps "which are not converted into a LAC by the perturbation" ?

The authors could explicitely state whether nuclear spin relaxation can also be described with this approach. Also, for adiabatic passage "the population adjust to the slow varation of the adiabatic eigenstates"; is that a coherent process ?

It would be helpful to explain in each case the basis chosen to write the initial density matrix. For example, in Eq. 20 polarisation operator are used, while in Eq. 29 populatin operators are used. Also the quantities M_I and M_S in Eq. 20 should be better defined. How to they relate to the populations ? What is their bounds ?

For the CP examples, the operators to move to the tilted frame, as well as the coupling terms, could be given explicitely.

Additional comments:

l. 64: the sentence "Such symmetry breaking can only occur under special conditions, which correspond to LACs" is a bit mysterious

l. 271: "Examples, in which basis rotation is taking place, are discussed below." Please clarify which examples

l. 491-510 are difficult to follow without a figure and/or a more detailed description.

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