Comment on mr-2021-39

Anonymous Referee #2

Referee comment on "Efficient polynomial analysis of magic-angle spinning sidebands and application to order parameter determination in anisotropic samples" by Günter Hempel et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-39-RC2, 2021

The paper under review proposes a polynomial analysis of MAS spinning sidebands to determine the chemical shielding tensor and the order parameter in anisotropic samples. MAS sideband analysis is typically performed by a procedure due to Herzfeld and Berger. This paper introduces an exact polynomial representation of SSB intensities to overcome the "far too complicated to be applied", in the words of the authors, Herzfeld-Berger relation. The application of the proposed method that is envisaged is for the determination of order parameters in polymers.

The first question that comes up is the justification that the polynomial evaluation will be appreciably faster than a numerical powder average of the expression that is routinely used. Secondly, it is not clear how the polynomial expression that is obtained is exact, as is claimed; it is an approximation to some order. That said, there are some interesting aspects to the paper. Taking sum and difference of positive and negative sidebands of a particular order is one such. Is this only true for polynomial expansion or is it general? So also is the use of symbolic manipulation programs for evaluating the coefficients.

Now to some nitty-gritty (ignoring the typos).

1. It is understandable that in successive rotations the last rotation of the previous rotation and the first rotation of the present can be combined because they are about the same axis. However, wouldn't the first rotation of the first and the last rotation of the last remain?

2. Because of performing rotations in the vector space spanned by the tensors, rotations are treated as a left multiplication with a 5 x 5 matrix. The advantage that this affords over bilinear matrix operations would depend on the number of multiplication and addition operations involved, and not on the size (storage is a minor factor).

3. In equation 25 (and may be a few others), the coefficients vary over orders of magnitude with some of the coefficients being extremely small. Are these small coefficients really significant?

4. In Figure 2, one find that the I+ intensity for the 12th order polynomial lies between 6 and 12. Increase the order would make it go further towards 2? That looks counter-inutitive.

5. In Figure 4, what are the triangles and what is the red curve?

6. Something is missing from the sentence starting at the end of line 321.

7. Why is the \delta of C1 and C2 in Table 2 different from that on line 374?

8. Equation 38 assumes that C2 and C5 are polarized identically despite the protons around them being two bonds apart in one case and three bonds apart in the other.

9. What is the origin of equation 39?