

Visualizing Distant Dipolar Field and Intermolecular Multiple Quantum Coherence Sequences

C. A. Corum¹, A. F. Gmitro^{1,2}

¹Optical Sciences Center, University of Arizona, Tucson, AZ, United States, ²Department of Radiology, Arizona Health Sciences Center, Tucson, AZ, United States

Motivation: Distant Dipolar Field or intermolecular multiple quantum coherence (DDF/iMQC) sequences are difficult to explain. They do not behave according to the common assumptions of the vector Bloch model. There are two major conceptual frameworks, classical and quantum, and the understanding of either requires a substantial level of mathematical knowledge. In order to make the concepts accessible to the non-mathematical or casual researcher a series of 3d animations has been developed, showing the states of transverse and longitudinal magnetization at each step of the CRAZED (COSY Revamped with Asymmetric Z Gradient Echo Detection) and related sequences.

Background: Deville¹ et al. first reported multiple spin echoes (MSEs) in ³He at low temperatures over 20 years ago and attributed them to the dipolar field from magnetization in the sample. They experimented with creating periodic magnetization in an otherwise homogenous sample. They also discovered that the form of the resulting signal equation could be simplified greatly if one assumed that the DC spatial component of magnetization was the dominant spatial Fourier component at equilibrium (usually a good assumption, even in a structured sample). Subsequently Bowtell² and collaborators reported observing MSEs in water at room temperature, opening the door to utilization of the DDF in solution NMR experiments and MRI. Warren³ et al. then interpreted the signal as due to intermolecular multiple quantum coherences (iMQCs) and developed single echo sequences.

Discussion: The CRAZED sequence consists in its simplest form of two RF pulses interspersed with two gradients and delays:

$$90^\circ - G - \tau - \beta^\circ - nG - |n| \tau - \text{echo}$$

The gradients are in the integer ratio n:1 and in the iMQC interpretation the “order” of the coherence during the period τ is determined by $|n|$, $n = 0$ corresponding to zero-quantum coherence; $n = 1, -1$ to single-quantum coherence (precessing transverse magnetization); $n = -2, 2$ to double quantum coherence; and larger n to higher orders. An echo is observed after delay $|n|\tau$, which for $n \neq -1$ contradicts the prediction of the vector Bloch model. Note that a good starting point of the pedagogical discussion is $n = -1$, $\beta = 180^\circ$, showing the CRAZED sequence as a generalization of the normal spin-echo sequence.

The essence of the CRAZED sequence is that spatially periodic z magnetization (Figures 1 and 2) is created by the subsequence:

$$90^\circ - G - \tau - \beta^\circ$$

This induces a Z-dependent change in the local precession frequency from its dipolar field. This leads to advances and retardations of the phase of the elliptical helix of the accompanying transverse magnetization. β determines how much transverse magnetization is rotated back to Z magnetization and how elliptical the transverse magnetization becomes; G (and its duration) determines the helix pitch. In the latter subsequence:

$$nG - |n| \tau - \text{echo}$$

the DDF from M_z first creates “harmonics” of the original transverse magnetization at multiples of the original helix pitch (Figures 3 and 4). These then require a different gradient, nG , to untwist. During the original τ delay, inhomogeneities also act on the transverse magnetization (not shown), so the $|n| \tau$ delay is necessary to refocus these (the process of generating harmonics has multiplied their effect). In the case $n = 0$ no untwisting is necessary, also explaining the inhomogeneity insensitivity of HOMOGENIZED^{4,5}.

Each step in the sequence is represented by the state of the helix, and its components. The transitions between steps are animated.

Many other phenomena can be visualized and explained. Enhanced diffusion weighting⁶ is visualized by noting the reduced M_z generated from attenuation of transverse magnetization before β . During the post β signal build period, the spatially modulated M_z itself decays, giving additional diffusion weighting insensitive to motion⁷. Interaction with periodicities in the object can also be included showing the cause of the “dips” in MSE sequences and novel contrast of DDF/iMQC based imaging sequences.

References:

1. G. Deville et al., *Phys. Rev. B*, 19(11):5666-5688, 1979
2. R. Bowtell et al., *Journal of Magnetic Resonance*, 88(3):641-651, 1990
3. Q. He et al., *The Journal of Chemical Physics*, 98(9):6779-6800, 1993
4. S. Vathyam, S. Lee, W. S. Warren, *Science* 272:92-96, 1996
5. C. Faber et al., *Journal of Magnetic Resonance*, 161(2): 265-274, 2003
6. J. Zhong et al., *Magnetic Resonance Imaging*, 19(1):33-39, 2001
7. S. D. Kennedy et al., ISMRM Proceedings, volume 11, talk 0581, 2003
8. F. M. Alessandri et al., *Journal of Magnetic Resonance*, 156(1):72-78, 2002

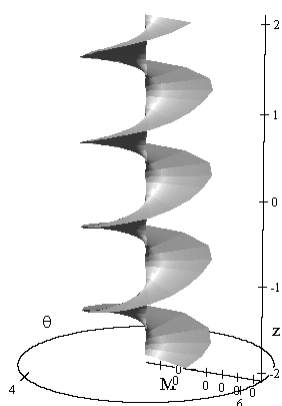


Fig. 1 – Helix formed from uniform sample magnetization density and applied grating after the β pulse

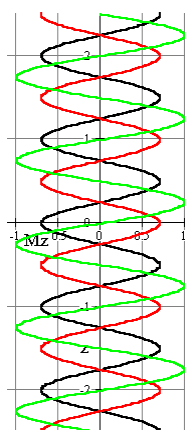


Fig. 2 – Helix components M_x , M_y , and M_z

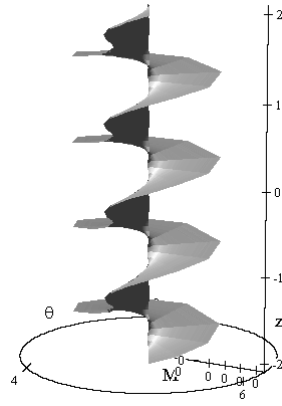


Fig. 3 – Helix components M_x and M_y after time τ , advanced or retarded by the DDF proportional to M_z .

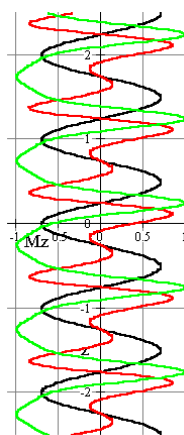


Fig. 4 – Both a DC term and a “harmonic” term have developed, in M_x and M_y , when untwisted they yield the zero and double-quantum echoes respectively.