

## Specialty area: MR Physics for Physicists

**Daniel F. Gochberg**

daniel.gochberg@vanderbilt.edu

### Highlights

- There are multiple ways to describe spins: classical magnetization vectors, bra-kets, density matrices, and product operators.
- Product operator evolution depends on the pulse sequence and coupling constants, and can be described in terms of quantum coherences.
- This evolution can be exploited to filter out uncoupled spins or to indirectly detect multiple quantum coherences not visible in the fid.

### Multiple quantum coherence, editing, and Multidimensional NMR

#### Target Audience

The target audience includes those familiar with a Bloch equation approach to modeling magnetization who have some familiarity with a quantum description of spins (perhaps from the previous two talks) and are looking for an introduction to multiple quantum sequences.

#### Objectives

This talk will explain how a spin state is represented, how it changes in time, and how to use this evolution to filter out uncoupled spins from the measured signal and to separate and indirectly detected spin evolution through 2D spectroscopy.

#### Introduction

The transverse magnetization precesses at the Larmor frequency, and this oscillation can be directly measured in the free induction decay (fid) signal. In contrast, multiple quantum coherences (MQCs) evolve at some multiple of the Larmor frequency (including zero), but this evolution frequency cannot be directly measured and is evident only through two dimension measurements. However, this difference in evolution frequency can be used to distinguish spins by their degree of coupling, and this filtering has practical applications.

In this class, we will discuss classical and quantum descriptions of the spin state, simplifying graphical representations, spin state evolution with time, and applications of multiple quantum filtering.

#### Representations

Spin states can be represented using classical magnetization vectors, bra-ket dirac notation, density matrices (1), and product operators (2). Magnetization vectors are simple and effective representations for isolated spins, but are not well suited to multiple quantum coherences. Bra-ket notation incorporates the limited measurement possibilities and inherent uncertainty of pure quantum states, but such states are not relevant for the bulk sample measurements in NMR and MRI. Density matrices incorporate the effects of an ensemble of many spins, and they reveal multiple quantum coherence effects, but their connection to the underlying spin evolution is sometimes opaque. Product operators decompose the density matrix into more easily

understandable basis operators, whose evolution and connection to the underlying spin characteristics is the subject of this talk. The two most widely used product operators are Cartesian (which connect to geometry) and spherical tensor (which connect to the time evolution).

## Evolution

A basic sequence that produces MQC is  $90_x$ - $\tau$ - $180_x$ - $\tau$ - $90_x$ - $t_1$ - $90_x$ . The first two pulses make up a simple spin echo sequence, and as such they refocus any field inhomogeneities or chemical shifts. During this preparation period, coupled spins evolve as  $I_z \rightarrow I_y \rightarrow 2I_xS_z$ . The  $90_x$  pulse then converts  $2I_xS_z$  into  $2I_xS_y$ . This MQC evolves during  $t_1$ , and can form the basis for filtering or can be indirectly detected via 2D measurements.

## 2D measurements

Most readers are already familiar with a simple 2D measurement: inversion recovery. In this case, the evolution of the z-magnetization is only revealed by a series of measurements, each with a different inversion time. At no point is the z-magnetization directly measured. Also note that the z-magnetization precesses at a frequency of zero, not the Larmor frequency of the directly measured magnetization. These same sequence characteristics appear in the 2D multi-quantum measurements, but with significantly more complex spin states and evolution.

## Applications

MQCs are produced in a wide range of pulse sequences and samples, and occur when there are motional restrictions or anisotropies, as in tissues (3), when water protons are separated by distances much greater than their diffusion distances (4), and when spins are connected via intramolecular coupling (5). These coherences can be used to distinguish coupled from uncoupled spins, or strongly coupled from weakly coupled spins. Homonuclear zero quantum coherences (ZQC), where spins precess at the difference in the resonant frequencies of the interacting spins, have the added benefit of being insensitive to inhomogeneities in the static field  $B_0$ , and hence can resolve peaks that may otherwise be blurred in conventional spectroscopy.

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3. Navon G, Shinar H, Eliav U, Seo Y. Multiquantum filters and order in tissues. *Nmr in Biomedicine* 2001;14(2):112-132.
4. Warren WS, Richter W, Andreotti AH, Farmer BT. Generation of Impossible Cross-Peaks between Bulk Water and Biomolecules in Solution Nmr. *Science* 1993;262(5142):2005-2009.
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