Multiple Quantum Coherence, Editing & Multidimensional NMR
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Nuclear magnetic resonance (NMR) which forms foundation of MRI, after all, is a quantum mechanical phenomenon. Even though in the imaging community we are mostly familiar with and most times use the so-called vector model to describe the MR signal as from a precessing bar magnet inside the magnetic field (not too much different from a spinning toy top in the earth's gravitation field), at a more fundamental level quantum mechanics should be used for NMR, and there are cases for which only invoking quantum mechanics can the complex interactions among nuclear spins be understood.

In soft tissues, bones or most systems we are interested in studying with MR (except water signal-only MRI), electrons around the nucleus shield it from the external magnetic field, causing **chemical shift** of resonance peaks. Electrons in the bonds between the nuclei mediate an interaction, resulting in **Scalar or J-coupling**, and split the signals according to the number of neighboring nuclei. The nuclei also interact directly through space via a dipole-dipole interaction, or **dipolar coupling**.

The phenomena of **multiple-quantum coherence** (MQC) not only provides a nice demonstration of the true quantum mechanical nature of NMR, applications of various MQC techniques also reveal many interesting structural and functional information in MRS and MRI. MQCs come from direct interactions among nuclear spins. MQCs are applicable not only to spin 1/2 systems such as for protons, but also to other spin $\geq$ 1/2 nuclei, such as sodioum (Na), an important nucleus in human body. The MQC signals can be induced by scalar couplings in isotropic solution, by intra-molecular dipolar couplings in anisotropic solution or solids, and by quadrupolar couplings in solid with spin $\geq$ 1/2 nucleus [1-5]. In anisotropic liquid such as liquid crystals, partial molecular alignment results in non-zero residual dipolar and quadrupolar interactions, leading to splitting of the resonance lines. In tissues such as tendons and vascular walls, the preferred alignment of water protons causes detectable dipolar interactions [6-9]. Multiple-quantum filtered (MQF) NMR spectroscopy, in particular double-quantum filtered (DQF), is called to reveal the splitting of spectral lines or orientational dependence of MR signals [6-9]. Furthermore, the measurement of dipolar coupling constant may provide useful information in structure studies and MRI. Magnetization transfer (MT) has also been accepted as an additional way to generate unique contrast for MRI [10-13]. The combination of DQF and MT (DQF-MT) provides a new MRI method especially useful for connective tissues as well as brain and spinal cord [6]. Recent works also elucidate that inter-molecular (among different molecules) MQC signals can be observed in a highly polarized system, such as in tissues. These peaks are resulted from dipolar interactions between distant nuclei in solution. In recent years, attention has been paid to the physical mechanisms and applications of inter-molecular MQCs in the NMR community [14-18]. Some new methods have been established in human MRI, and high-resolution MRS in inhomogeneous field.

To explore complex and rich information provided by all major interactions among resonance spins, and often to simply the results, we often resort to **Editing** and **Multidimensional NMR** [19-21]. Editing refers to processes in which signals acquired with different parameters are added/subtracted to eliminate certain signals while enhancing others. Signals can be either excited selectively, or allow accumulation of phases for different spin spices. In multidimensional NMR, information is acquired to separately represent different nuclear interactions onto different spectral axis. For example, in 2D-NMR, 3 axes are presented, with intensity vs. frequency 1 (i.e. chemical shift) in one axis, and intensity vs. frequency 2 (i.e. due to scalar coupling) in another axis. The two major advantages of multidimensional NMR are:
- Improved resolution: Signals are spread over a surface (2D) or in a three-dimensional space (for 3D, 4D NMR).
- Magnetization transfer: Signals result from the interaction between nuclei. That can be interactions through bond (via J-coupling) or through space (via NOE).
Taken together this eases the interpretation and the assignment of the spectra considerably.

In this presentation, we will first take a scalar coupled two-spin system as an example to illustrate the formation of multiple-quantum coherences. We will then look at the directly dipole-dipole coupled spins and distant dipole-dipole interactions, and demonstrate how they can lead to signals that resemble MQCs in scalar coupled spins. Basic analytical tools for the treatment of the phenomena will be presented. Multiple-deminsional MR and editing techniques will be illustrated. Some important recent applications of the discussed effects and techniques will be presented.

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