Analytical tool for *in vivo* magnetic resonance signals

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Many scientists, including MagLab users, widely utilize triple quantum (TQ) magnetic resonance (MR) signals in their research. For *in vivo* experiments, such signals come mainly from sodium and potassium ions which interact with negatively charged groups of macromolecules, mainly proteins. *MR signals appearing as a result of protein interactions indicate changes of intracellular ion content* in vivo *during diseases and drug administration*. These signals can be efficiently extracted from other ions by using TQ effects. Note that the behavior of the MR magnetization in the presence of spin >1/2 is not possible to explain by the simple vector model routinely used for proton MR.

The computer based tool is presented to describe and visualize the results of MR signal evolution *in vivo* in multi-pulse MR experiments. *The system of theoretical equations describes MR signal evolution exactly without any approximation and needs to be constructed only once, which is then valid for any interval in the pulse sequence as well as for any spin value*. The theoretical calculations are illustrated using the power of "Mathematica" software (Wolfram Inc.) for traditional TQ radio frequency (RF) pulse sequence (see Figure). The results of calculations can be visualized, noting that MR magnetization must remain unchanged during a parity transformation, i.e. changing the sign of all coordinates.

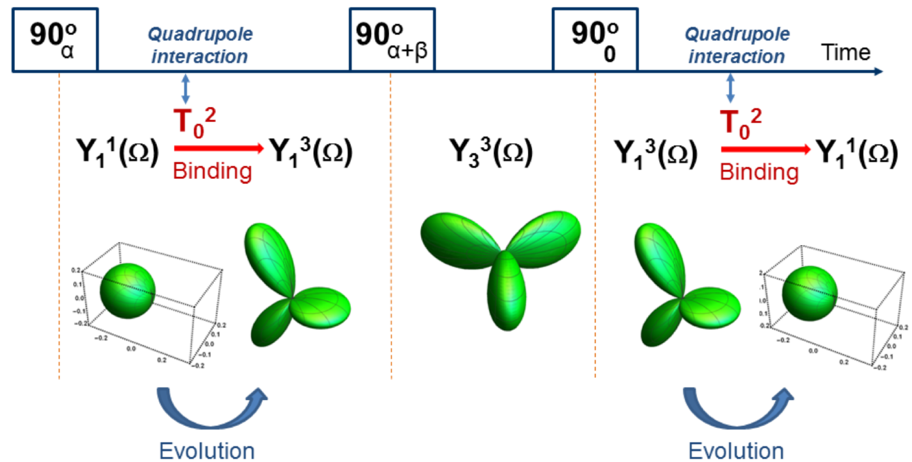

Figure: The analytical tool is illustrated by visualization of the triple quantum (TR) magnetic resonance (RF) signals inside the traditional TQ RF pulse sequence. Spherical harmonics $Y_m^L(\mathbf{\Omega})$, which are presented also graphically (green color), represent the changes of nuclear magnetization for spin = 3/2, as created by RF pulses in the presence of the quadrupole interaction indicated by T_0^2. The central goal of the TQ pulse sequence is to create MR magnetization in the state of $Y_3^3(\mathbf{\Omega})$. Note that all states of the magnetization $Y_m^3(\mathbf{\Omega})$ for any "m" are not observable in experiments and can be represented only mathematically. At the end of the TQ pulse sequence the quadrupole interaction is needed again to evolve the unobservable state $Y_1^3(\mathbf{\Omega})$ into observable MR magnetization state presented by $Y_1^1(\mathbf{\Omega})$.

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