Selective Rotation Pulses calculated with an Inverse Scattering Algorithm

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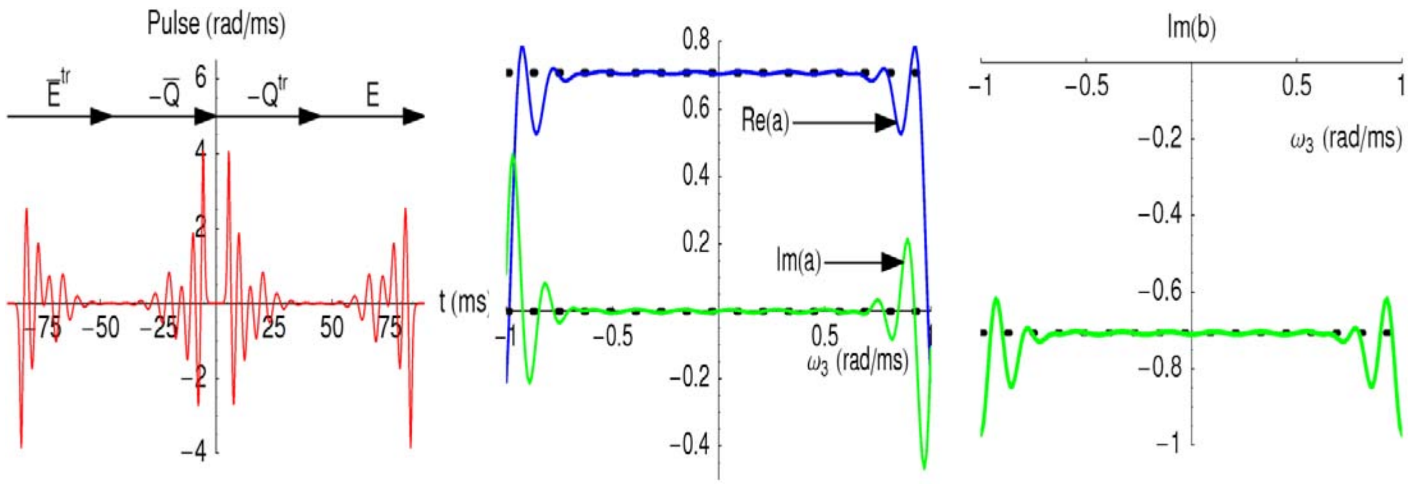
Introduction: A new approach to determine arbitrarily accurate selective rotation pulses is introduced. The group of selective rotation pulses include the "universal" pulses[1], which provide a uniform spin rotation (within a given frequency range or slice), irrespective of their initial states. This makes them useful for applications such as NMR imaging or NMR spectroscopy in inhomogeneous B_0-fields. The purpose was to make this group of pulses easily and generally accessible.

Theory: As recently shown[2], an arbitrary selective rotation pulse can be generally constructed by two point-to-point (PP) pulses $R \cdot \bar{R}^{tr}$ ($\bar{R}^{tr}$ is the phase-reversed $^{-}$ and time-reversed ^{tr} counterpart of R). Decomposing each of these PP pulses into two sub-pulses E and Q,

$$R \cdot \bar{R}^{tr} = (E \cdot Q^{tr}) \cdot (-\bar{Q} \cdot \bar{E}^{tr})$$

enables an inverse scattering algorithm to determine each sub-pulse separately. The denominator of the stereographic projection[3] of the desired magnetization responses of E and Q can be approximated as accurately as necessary by a rational function (e.g. a Butterworth function). A low order approximation (with a corresponding low quality of the magnetization response) leads to a closed-form expression for the sub-pulses. Using higher order approximations, arbitrarily accurate selective rotation pulses are (numerically) found.

Results: The (semi-infinitely long) sub-pulses were truncated and joined together. Figure 1 shows a numerically calculated 90° selective rotation pulse $R \cdot \bar{R}^{tr}$ (A) and the corresponding spinor responses (B) and (C). The knowledge of the spinor coefficients a and b is equivalent to the knowledge of the rotational response.



(A) (B) (C)

Figure 1: A $90_x°$ selective (between ± 160 Hz) rotation pulse (A), which rotates all spins about the x-axis, irrespectively of their initial orientations. Figures (B) and (C) show the corresponding spinor response within the slice $-1 < \omega_3 < 1$ rad/ms. The dashed lines are the desired values of a perfect spin rotation.

By increasing the approximation level the desired spinor response can be reached as closely as possible. Generally a higher approximation level causes a longer total pulse duration. To avoid excessive pulse durations more efficient polynomials can be used for the approximation.

Discussion: A universal method to calculate selective rotation pulses was introduced. This opens the door for the general use of these pulses in all fields of NMR application, suffering from B_0-inhomogeneities. Other applications include spatially selective coherence transfer[4] or qubit manipulations[5] in optical quantum computers.

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References: [1] Geen, JMR, (1991), 93:93-141; [2] Luy, JMR, (2005), 179-186; [3] Bloch, (1940), Phy.Rev., 70:460; [4] Shen, (2003), JMR, 163:73-80; [5] Cummins, (2001), JMR, 148:338-342;