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Selective rotation pulses calculated with an inverse scattering algorithm

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Abstract

Selective rotation pulses cause magnetization within a given frequency range (or slice) to undergo a specified rotation, about a specified axis. Magnetization outside this slice remains unaffected if it is initially along the z axis. It has previously been shown that the design of such pulses can be reduced to the design of selective "point-to-point" pulses, which rotate magnetization within the slice from the y axis. By decomposing the point-to-point pulses into two sub-pulses, it is shown that an inverse scattering algorithm for selective pulse design can be used to calculate selective rotation pulses with any desired spinor response, subject to the constraint that the second spinor component have constant phase across the slice. The design of selective refocusing pulses can be treated specially, requiring the calculation, by the same inverse scattering algorithm, of a single sub-pulse.

Keywords: Selective rotation pulses; Universal rotations; General rotation pulses; Selective refocusing pulses; Inverse scattering; Spinors

1. Introduction

Selective rotation pulses are an interesting class of pulses which effect a given rotation of magnetization vectors within a frequency band, irrespective of their initial orientations. For example, a 90_y° selective rotation pulse would rotate all magnetization within a given band by 90 degrees about the y axis. Within this frequency band, magnetization initially aligned with the z axis would end up aligned with the x axis. Magnetization initially aligned with the x axis would end up along the $-z$ axis. Magnetization outside this frequency band would not receive this rotation: it is usual to require that it be rotated only about the z axis.

Selective rotation pulses are known by a variety of names, including "type A" [1], "R-type" [2],[1] "general rotation", or "universal" (UR) pulses [3,4]. Selective rotation pulses that provide a *uniform* rotation within the selected band (and rotation only about the z axis outside) are of particular interest, as they are the equivalent of hard pulses within this band. They can therefore be used to achieve spatially selective coherence transfer [5] and be used to implement qubit manipulation in NMR and optical quantum computers [6,7].

Selective rotation pulses appear to be much more difficult to calculate than usual selective pulses, which are required to rotate magnetization, within a band of frequencies, from a fixed point [normally (0,0,1)] to some final state, as a function of frequency offset. These latter pulses will be referred to here as selective point-to-point (PP) [8] pulses [as for selective rotation pulses, "selective" should be taken to mean that outside of a given frequency band, magnetization is rotated only about z, so initial magnetization $(0,0,1)$ remains at $(0,0,1)$].

Indeed it has not been clear whether it is possible to obtain arbitrarily accurate selective rotation pulses, in contrast to selective PP pulses which can be calculated exactly using the (equivalent) methods of inverse scattering [9], Schur-type iteration [10–12] or the Shinnar-Le Roux algorithm [13,14].

This question is answered in this paper. It is shown how inverse scattering theory can be used to calculate arbitrarily specified selective rotation pulses (to within a constraint that will be described).

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[1] More accurately, in the notation of [1], type A within the selected slice, and type B2 outside (or [2] R-type within, M-type outside).

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2. Theory

2.1. Reducing the selective rotation problem to a point-to-point problem

A key result that enables the exact calculation of selective rotation pulses is from [8]. It is convenient to express this result in terms of spinors, which provide a simple way of representing rotations. In particular, a rotation R of angle θ about the (unit) vector (n_x, n_y, n_z) can be represented by the 2×2 matrix [4,15,16]

$$U = \begin{pmatrix} \cos(\theta/2) - \mathrm{i}n_z \sin(\theta/2) & -\mathrm{i}\sin(\theta/2)(n_x - in_y) \\ -\mathrm{i}\sin(\theta/2)(n_x + \mathrm{i}n_y) & \cos(\theta/2) + \mathrm{i}n_z \sin(\theta/2) \end{pmatrix}. \quad (1)$$

It is sufficient to write down just the components in the first column of U (since the second column can be deduced from it):

$$u = (\cos(\theta/2) - \mathrm{i}n_z \sin(\theta/2), -\mathrm{i}\sin(\theta/2)(n_x + \mathrm{i}n_y)) \quad (2)$$

and u is the spinor representing this rotation.

Furthermore, let $\mathbf{v} = (v_x, v_y, v_z)$ be a vector. The effect of rotating $\mathbf{v}$ by R to $\mathbf{v}'$ is determined by evaluating

$$V' = UVU^{-1}, \quad (3)$$

where

$$V = \begin{pmatrix} v_z & v_x - \mathrm{i}v_y \\ v_x + \mathrm{i}v_y & -v_z \end{pmatrix} \quad (4)$$

and U^{-1} (the inverse of U) is obtained by substituting θ by $-\theta$ in Eq. (1). Then the rotated vector $\mathbf{v}'$ can be deduced, since V' must equal

$$V' = \begin{pmatrix} v'_z & v'_x - \mathrm{i}v'_y \\ v'_x + \mathrm{i}v'_y & -v'_z \end{pmatrix}. \quad (5)$$

Consider the special case when $\mathbf{v} = (0,1,0)$. Write $u = (a, b)$, and hence

$$U = \begin{pmatrix} a & -b^{\star} \\ b & a^{\star} \end{pmatrix}, \quad U^{-1} = \begin{pmatrix} a^{\star} & b^{\star} \\ -b & a \end{pmatrix}, \quad (6)$$

where * denotes the complex conjugate. Then Eqs. (3)–(5) imply that

$$v'_x + \mathrm{i}v'_y = \mathrm{i}(a^{\star 2} + b^2), \quad v'_z = \mathrm{i}(ab - a^{\star}b^{\star}). \quad (7)$$

Now suppose $P(t)$ is a pulse that rotates a magnetization vector by the rotation R above (i.e., the rotation can be represented by u or U above). Using the notation of [8], where $^{\mathrm{tr}}$ denotes time-reversed and $^{-}$ denotes phase-reversed, let $\bar{P}^{\mathrm{tr}}$ be the time- and phase-reversed pulse $P^{\star}(-t)$. Then [1] the response of $\bar{P}^{\mathrm{tr}}$ can be represented by a matrix $\bar{U}^{\mathrm{tr}}$, or by an equivalent spinor $\bar{u}^{\mathrm{tr}}$, where for example,

$$\bar{u}^{\mathrm{tr}} = (a, -b^{\star}). \quad (8)$$

The effect of pulse $P \cdot \bar{P}^{\mathrm{tr}}$ (i.e., $\bar{P}^{\mathrm{tr}}$ followed by P) is then

$$S = U\bar{U}^{\mathrm{tr}} = \begin{pmatrix} a^2 + b^{\star 2} & ab - a^{\star}b^{\star} \\ ab - a^{\star}b^{\star} & a^{\star 2} + b^2 \end{pmatrix}, \quad (9)$$

i.e., it can be represented by the spinor

$$s = (a^2 + b^{\star 2}, ab - a^{\star}b^{\star}). \quad (10)$$

Comparing Eqs. (7) and (10), it can be concluded that if P rotates a magnetization vector initially at $(0,1,0)$ to (m_x, m_y, m_z), then the composite pulse $P \cdot \bar{P}^{\mathrm{tr}}$ has spinor response

$$s = (\mathrm{i}m^{\star}, -\mathrm{i}m_z), \quad (11)$$

where $m = m_x + \mathrm{i}m_y$. It is therefore possible to design a selective rotation pulse with any desired spinor response as a function of frequency offset ω_3,

$$s_{\mathrm{des}}(\omega_3) = (a_{\mathrm{des}}(\omega_3), b_{\mathrm{des}}(\omega_3)) \quad (12)$$

(with the constraint that the second component of the spinor is always imaginary[2]) provided that it is possible to design selective PP pulses that rotate magnetization within the selected slice from $(0,1,0)$ to (m_x, m_y, m_z) where

$$\mathrm{i}(m_x - \mathrm{i}m_y) = a_{\mathrm{des}}, \text{ and } -\mathrm{i}m_z = b_{\mathrm{des}}. \quad (13)$$

This reduction of the selective rotation problem to a PP problem was the key result of [8]. How to analytically solve the PP problem has not previously been described, and this is now done.

2.2. Solving the point-to-point problem

2.2.1. Pulses Q and E

The required magnetization response (13) of pulse P can be accomplished by requiring that pulse P must (inside the slice) (a) rotate initial magnetization $(0,1,0)$ to $(0,0,1)$ and then (b) rotate magnetization $(0,0,1)$ to (m_x, m_y, m_z) of Eq. (13). Outside the slice, it is sufficient to require that magnetization $(0,0,1)$ remain at $(0,0,1)$ after both steps.

Processes (a) and (b) can be achieved by appropriately chosen pulses.

Let Q be a selective PP pulse that rotates magnetization $(0,0,1)$ to $(0,1,0)$ within the selected slice. It is known [8] (see also [17]) that the pulse $-Q(-t) = -Q^{\mathrm{tr}}$ will rotate magnetization $(0,1,0)$ to $(0,0,1)$ within the selected slice, provided the slice is symmetrically placed about $\omega_3 = 0$. It is easy to verify this with the spinor formalism of Section 2.1,[3] and also to verify that outside the slice, magnetization $(0,0,1)$ will stay at $(0,0,1)$ after pulse $-Q^{\mathrm{tr}}$.

Pulse P can therefore be constructed as pulse $-Q^{\mathrm{tr}}$ followed by the selective excitation pulse E that (within the selected slice) rotates magnetization $(0,0,1)$ to (m_x, m_y, m_z) satisfying Eq. (13). Then $P = E \cdot -Q^{\mathrm{tr}}$ has properties (a), (b) listed above.

[2] Hence, the rotation axis must always be in the x–z plane. It is possible to rotate this plane by using the phase-shifted pulse $(P \cdot \bar{P}^{\mathrm{tr}})e^{i\phi}$ [8].

[3] Using the fact that if the spinor response of Q at frequency offset ω_3 is $(a_Q(\omega_3), b_Q(\omega_3))$, the spinor response of $-Q^{\mathrm{tr}}$ is $(a_Q^{\star}(-\omega_3), -b_Q(-\omega_3))$.

The selective rotation pulse, can then be written down:

$$P \cdot \bar{P}^{\mathrm{tr}} = E \cdot -Q^{\mathrm{tr}} \cdot -\bar{Q} \cdot \bar{E}^{\mathrm{tr}}, \tag{14}$$

and this will induce a selective rotation given by the spinor of Eqs. (12) and (13). In fact, usually the Q and E pulses can be "spliced" together over some interval, as illustrated in an example below.

2.2.2. Calculating pulses Q and E

Selective PP pulses Q and E used to construct the selective rotation pulses can be calculated with inverse scattering theory. The method described in [9] is fairly compact and simple. It is applicable when the initial magnetization is (0,0,1) for all frequency offsets, as is the case for pulses Q and E.

The desired magnetization response $(m_x^{\mathrm{des}}, m_y^{\mathrm{des}}, m_z^{\mathrm{des}})$ of the selective PP pulse needs to be expressed as the stereographic projection

$$\Gamma_{\mathrm{des}} = \frac{m_x^{\mathrm{des}} + \mathrm{i} m_y^{\mathrm{des}}}{1 + m_z^{\mathrm{des}}}. \tag{15}$$

Furthermore, Γ_{des} needs to be a rational polynomial in frequency offset ω_3, i.e., have the form

$$\Gamma_{\mathrm{des}}(\omega_3) = \alpha \frac{\prod_{j=0}^{m-1} \omega_3 - z_j}{\prod_{j=0}^{n-1} \omega_3 - p_j}, \tag{16}$$

where $n > m$ (which ensures that $\Gamma_{\mathrm{des}} \to 0$ as $\omega_3 \to \pm\infty$). Functions that are not in rational polynomial form can usually be approximated as such to arbitrarily high precision using, for example, Padé or minimax approximation [18].

Let ζ_j, $j = 0, \ldots, 2n-1$, solve

$$\Gamma_{\mathrm{des}}(\zeta_j)\Gamma_{\mathrm{des}}^{\star}(\zeta_j^{\star}) + 1 = 0, \tag{17}$$

noting that if ζ_j is a solution, so is $\zeta_j^{\star}$. Then solve the linear matrix equation

$$\left.\begin{array}{l} \sum_{j=0}^{2n-1} \frac{\mathrm{e}^{-(\mathrm{i}/2)\zeta_j t}}{\zeta_j - p_k} f_j = 0 \\ \mathrm{i} \sum_{j=0}^{2n-1} \frac{\mathrm{e}^{(\mathrm{i}/2)\zeta_j t}}{\zeta_j - p_k^{\star}} \Gamma_{\mathrm{des}}(\zeta_j) f_j = 1 \end{array}\right\} k = 0, \ldots, n-1, \tag{18}$$

for $f_j(t)$, $j = 0, \ldots, 2n-1$. Finally, the pulse (in units of angular frequency) with response Γ_{des} at $t = 0$ is

$$\omega(t) = -2\mathrm{i} \sum_{j=0}^{2n-1} f_j(t) \mathrm{e}^{-(\mathrm{i}/2)\zeta_j t} \tag{19}$$

assuming without loss of generality that the pulse runs from $t = -\infty$ to $t = 0$.

For pulse Q, the stereographic projection of its desired magnetization response is [Eq. (15)]

$$\Gamma_Q = \begin{cases} \mathrm{i} & \text{for } |\omega_3| < 1 \text{ rad/ms}, \\ 0 & \text{otherwise}, \end{cases} \tag{20}$$

assuming, without loss of generality, that the slice runs over the interval $-1 < \omega_3 < 1$ rad/ms (i.e., between ±160 Hz).

Γ_Q can be approximated by the Butterworth function

$$\Gamma_{\mathrm{des}} = \frac{\mathrm{i}\tan\phi}{1 + \omega_3^{2r}} = \mathrm{i}\tan\phi \frac{1}{\prod_{j=0}^{2r-1} \omega_3 - p_j}, \tag{21}$$

where $\phi = \pi/4$ (i.e., $\tan\phi = 1$), and $p_j = \exp[\mathrm{i}\pi/(2r)]\exp(\mathrm{i}j\pi/r)$ are the $2r$th roots of -1.[4] Here r is a positive integer. The greater the value of r, the closer the Butterworth function gets to the desired response. Other functions, such as Chebyshev rational polynomials can also be used to approximate Γ_Q [19].

To calculate the ζ_j, note that Γ_{des} of Eq. (21) satisfies

$$\Gamma_{\mathrm{des}}(\omega_3) = -\Gamma_{\mathrm{des}}^{\star}(\omega_3^{\star}) \tag{22}$$

and so Eq. (17) becomes $\Gamma_{\mathrm{des}}(\zeta_j) = \pm 1$. Let ζ_j^+ ($j = 0, \ldots, 2r-1$) solve

$$\Gamma_{\mathrm{des}}(\zeta_j^+) = 1. \tag{23}$$

Then $\zeta_j^- \equiv \zeta_j^{+\star}$ solves $\Gamma_{\mathrm{des}}(\zeta_j^-) = -1$. Therefore, the set $\{\zeta_j\}$ equals

$$\{\zeta_j\} = \{\zeta_0^+, \ldots, \zeta_{2r-1}^+; \zeta_0^{+\star}, \ldots, \zeta_{2r-1}^{+\star}\}. \tag{24}$$

For Γ_{des} of Eq. (21),

$$\begin{aligned} \{\zeta_j\} = \{ & (\sec\phi)^{1/(2r)} \mathrm{e}^{\mathrm{i}(\pi-\phi)/(2r)} \mathrm{e}^{\mathrm{i}k\pi/r}, k = 0, \ldots, 2r-1; \\ & (\sec\phi)^{1/(2r)} \mathrm{e}^{-\mathrm{i}(\pi-\phi)/(2r)} \mathrm{e}^{\mathrm{i}k\pi/r}, k = 0, \ldots, 2r-1\}. \end{aligned} \tag{25}$$

Once the p_j and ζ_j are known, Eq. (18) can be solved to evaluate functions $f_j(t)$ over a range of values of t (with $t < 0$), and hence the RF pulse Q can be calculated (19). In general, these steps must be performed numerically, although a closed-form expression does exist when $r = 1$ (see Example 4.1 below).

3. Refocusing pulses

The method of Section 2 can be used to design selective rotation pulses with arbitrarily specified spinor response inside the selected slice (to within the constraint described). Such rotation pulses can be decomposed into four sub-pulses: E, $-Q^{\mathrm{tr}}$, $-\bar{Q}$, and $\bar{E}^{\mathrm{tr}}$. However, the special (and important) case of designing selective refocusing pulses can be solved by a different method, which requires only two sub-pulses.

A selective refocusing pulse should rotate all magnetization within a slice by 180° about a fixed axis in the transverse plane (which can be chosen to be the x axis without loss of generality). Outside the slice, magnetization should be rotated only about the z axis. Then Eq. (2) shows that the desired spinor response has second component

[4] It is convenient later to consider Eq. (21) where $\phi \neq \pi/4$, hence this form with general ϕ is maintained.

$$b = \begin{cases} -i & \text{inside the slice} \\ 0 & \text{outside.} \end{cases} \tag{26}$$

It is not necessary to specify the first spinor component, a. The spinor components always satisfy $|a|^2 + |b|^2 = 1$, and therefore if b is chosen as in (26), then a automatically has the form that will give the desired spinor response. This extra freedom over the general case, i.e., the fact that only b needs to be specified, allows refocusing pulses to be calculated more easily than general selective rotation pulses.

Suppose pulse R is a PP pulse that, given initial magnetization $(0,0,1)$, produces a magnetization response (m_x, m_y, m_z) such that the stereographic projection $\Gamma = (m_x + \mathrm{i}m_y)/(1 + m_z)$ has the form

$$\Gamma = \frac{B}{\omega_3^r + \mathrm{i}B}, \tag{27}$$

where $r > 0$ is an integer, and B is a polynomial in ω_3 of order $r - 1$. Then the spinor response of R followed by $\bar{R}^{\mathrm{tr}} = R^{\star}(-t)$ has second component [20]

$$b = \frac{\Gamma - \Gamma^{\star}}{1 + |\Gamma|^2}. \tag{28}$$

Substituting Eq. (27) into this expression gives (assuming ω_3 is real)

$$b = -\mathrm{i}\frac{2|B|^2 + \mathrm{i}\omega_3^r(B - B^{\star})}{\omega_3^{2r} + 2|B|^2 + \mathrm{i}\omega_3^r(B - B^{\star})}. \tag{29}$$

Therefore, if B is chosen such that

$$2|B|^2 + \mathrm{i}\omega_3^r(B - B^{\star}) = 1, \tag{30}$$

then

$$b = \frac{-\mathrm{i}}{1 + \omega_3^{2r}}. \tag{31}$$

Similarly to Eqs. (20) and (21), this provides a Butterworth approximation to the desired b response (26), assuming the slice runs over the interval $-1 < \omega_3 < 1$ rad/ms.

Finding polynomials B that satisfy (30) is fairly straightforward: see examples 4.3 and 4.4. Given B, the pulse R with stereographic projection (27) can be found via the algorithm described in Section 2.2.2, and then the refocusing pulse is $\bar{R}^{\mathrm{tr}} \cdot R$.

4. Examples

4.1. 90_x° selective rotation (closed-form example, r = 1)

Selective rotation pulses are commonly required to rotate all magnetization within the selected slice by 90° about the x axis.

Therefore [Eq. (2) with $\theta = \pi/2$ and $(n_x, n_y, n_z) = (1,0,0)$] the desired spinor response of the selective rotation pulse is

$$s_{\mathrm{des}}(\omega_3) = (1/\sqrt{2}, -\mathrm{i}/\sqrt{2}) \tag{32}$$

within the selected slice (assumed as in Section 2.2.2 to run over the interval $-1 < \omega_3 < 1$ rad/ms).

Eqs. (11)–(13) then show that we need to find the selective pulse P that rotates magnetization in the selected slice from $(0,1,0)$ to (m_x, m_y, m_z), where

$$\mathrm{i}(m_x - \mathrm{i}m_y) = a_{\mathrm{des}} = 1/\sqrt{2}, \quad -\mathrm{i}m_z = b_{\mathrm{des}} = -\mathrm{i}/\sqrt{2}, \tag{33}$$

i.e.,

$$(m_x, m_y, m_z) = (0, 1/\sqrt{2}, 1/\sqrt{2}). \tag{34}$$

From Section 2.2.1, finding pulse P is reduced to finding pulse Q that rotates magnetization within the selected slice from $(0,0,1)$ to $(0,1,0)$ and finding pulse E that rotates magnetization in the slice from $(0,0,1)$ to (m_x, m_y, m_z) of Eq. (34).

Pulse Q can be calculated by following the steps in Section 2.2.2. Assume that a Butterworth function (21) of order $2r$ is used to approximate Γ_{Q} [Eq. (20)]. The parameter r would usually be taken as large as possible (as this improves the approximation). The case $r = 1$ is of interest, however, as a closed-form expression for the pulse can then be found. It is (in units of rad/ms)

$$Q(t) = \frac{-4\alpha_{\mathrm{i}} \operatorname{sech} \alpha_{\mathrm{i}}t\left[\sin \alpha_{\mathrm{r}}t + \frac{\alpha_{\mathrm{i}}}{\alpha_{\mathrm{r}}} \cos \alpha_{\mathrm{r}}t \tanh \alpha_{\mathrm{i}}t\right]}{1 + \left[\frac{\alpha_{\mathrm{i}}}{\alpha_{\mathrm{r}}} \cos \alpha_{\mathrm{r}}t \operatorname{sech} \alpha_{\mathrm{i}}t\right]^2}, \tag{35}$$

for $t < 0$, where α_{r} and α_{i} are the real and imaginary parts of

$$\alpha = \mathrm{i}e^{-\mathrm{i}\phi/2}\sqrt{\sec \phi}, \tag{36}$$

with ϕ the same parameter as in Eq. (21), i.e., $\phi = \pi/4$.

Pulse E can be found by noting that its desired response, written as a stereographic projection, is [Eqs. (15), (34)]

$$\Gamma_E = \begin{cases} \frac{\mathrm{i}/\sqrt{2}}{1+1/\sqrt{2}} = \mathrm{i}\tan\frac{\pi}{8} & \text{for } |\omega_3| < 1 \\ 0 & \text{otherwise.} \end{cases} \tag{37}$$

Just as for Γ_Q, this can be approximated by the Butterworth function of Eq. (21), but now with $\phi = \pi/8$. Therefore, if again r is chosen to equal 1, the pulse E has exactly the same form as Q in Eqs. (35), (36) but with $\phi = \pi/8$.[5]

The selective rotation pulse is then [Eq. (14)]

$$E \cdot -Q^{\mathrm{tr}} \cdot -\bar{Q} \cdot \bar{E}^{\mathrm{tr}}, \tag{38}$$

and this is shown in Fig. 1. Since pulses calculated by the method of Section 2.2.2 are always (semi-)infinitely long (i.e., in general, they can be non-zero for all $t < 0$), the pulses Q and E had to be truncated, i.e., set to zero for $t < -T$ before joining together according to (38).

The time T was chosen equal to 10 ms, but could be chosen shorter if it was necessary to reduce the total pulse duration. Another strategy to reduce the pulse duration is to splice the pulses together, i.e., instead of playing out

[5] In general, for a θ-selective rotation pulse, ϕ should equal $(\pi - \theta)/4$ for pulse E.

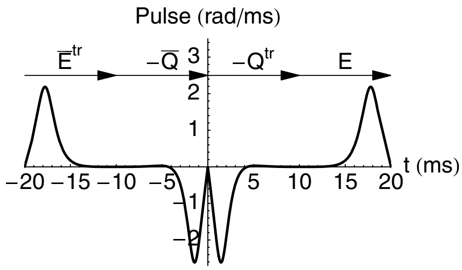

Fig. 1. Selective rotation pulse of Example 4.1, designed to produce a $90_x°$ rotation of magnetization within the slice $-1 < \omega_3 < 1$ rad/ms (i.e., between ±160 Hz). The individual components of the pulse ($\bar{E}^{tr}$ etc.) are indicated.

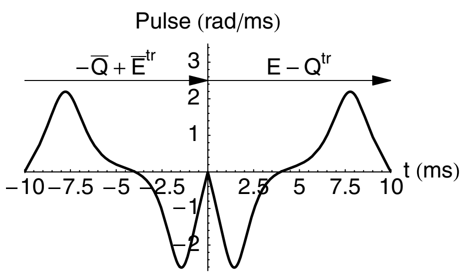

Fig. 2. Selective rotation pulse of Fig. 1, but the sub-pulses $\bar{E}^{tr}$ and $-\bar{Q}$ have been spliced together over their whole durations (similarly for $-Q^{tr}$ and E).

pulse $-Q^{tr}$ and then E, pulse E starts before the end of $-Q^{tr}$: where they overlap, the sum of the two pulses is used. The same splicing would need to be done to $\bar{E}^{tr}$ and $-\bar{Q}$ to maintain the pulse symmetry.

In this example, it is possible to splice the pulses together over their whole durations, giving rise to the selective rotation pulse of Fig. 2.

The spinor response to the spliced pulse of Fig. 2 was calculated[6] over the slice $-1 < \omega_3 < 1$ rad/ms, and compared to the desired response [Eq. (32)].

Outside this slice, the magnetization response to the pulse was calculated (assuming an initial magnetization along the z axis), and compared to the desired value (which is that the magnetization remains along the z axis). The magnetization response was not calculated inside the slice as no assumptions were made as to the initial magnetization of any spins inside the slice. The spinor response within the slice provides more information than the magnetization response, since the latter requires knowledge of the initial magnetization of spins, whereas the former does not.

Fig. 3 shows the spinor and magnetization responses to this pulse, together with the desired values (they are similar to the responses to the unspliced pulse of Fig. 1). Although the pulse is very easy to calculate (its sub-pulses have been written down in closed-form), the responses are less than ideal. The next example illustrates the improvement that follows choosing a larger value of r.

4.2. $90_x°$ selective rotation ($r = 6$)

When $r > 1$ in Eq. (21), it is easier to solve Eq. (18) numerically over a set of t values than to attempt to find a closed-form solution. Assuming the same desired spinor response [Eq. (32)] as in the previous example, and the same Butterworth approximation (21), this was done for $r = 6$, and with $\phi = \pi/4$ to give the pulse Q and $\phi = \pi/8$ to give the pulse E.

The (unspliced) pulse, with each sub-pulse truncated to a duration $T = 45$ ms, is shown in Fig. 4. The spinor response to this pulse within the slice $-1 < \omega_3 < 1$ rad/ms was calculated, together with the m_z response outside the slice (assuming magnetization initially along the z axis). These responses are shown in Fig. 5. They are compared with the desired values, still given by Eq. (32) inside the slice, and $m_z = 1$ outside the slice.

Increasing r improves the quality of the response, but at a cost of increased pulse duration. As in the previous example, reducing T or splicing (overlapping $-Q^{tr}$ and E by $T/2$, and similarly for $\bar{E}^{tr}$ and $-\bar{Q}$, works well) could be used, or an optimized choice of rational polynomial could be used instead of the Butterworth function of Eq. (21), if the overall pulse duration was excessive.

4.3. $180_x°$ selective rotation ($r = 1$)

As described in Section 3, selective refocusing pulses whose spinor response has second component

$$b = \frac{-\mathrm{i}}{1 + \omega_3^{2r}} \tag{39}$$

can be calculated by first solving the polynomial equation Eq. (30),

$$2|B|^2 + \mathrm{i}\omega_3^r(B - B^{\star}) = 1, \tag{40}$$

where B is a polynomial in ω_3 of order $r - 1$. The equation must be true for all ω_3, and hence each coefficient of ω_3 can be examined separately.

For $r = 1$, B is just a constant. This yields the equations

$$2|B|^2 = 1 \text{ and } B = B^{\star}. \tag{41}$$

Therefore

$$B = \pm 1/\sqrt{2} \tag{42}$$

and so the desired stereographic projection for pulse R is [Eq. (27)]

$$\Gamma = \frac{\pm 1/\sqrt{2}}{\omega_3 \pm \mathrm{i}/\sqrt{2}}. \tag{43}$$

There are therefore two possible choices of Γ. It can be made unique by insisting that it has no poles in the upper

[6] The spinor responses to all the pulses in these examples were calculated by numerically integrating the spinor equation of motion [12] over the given range of frequency offsets.

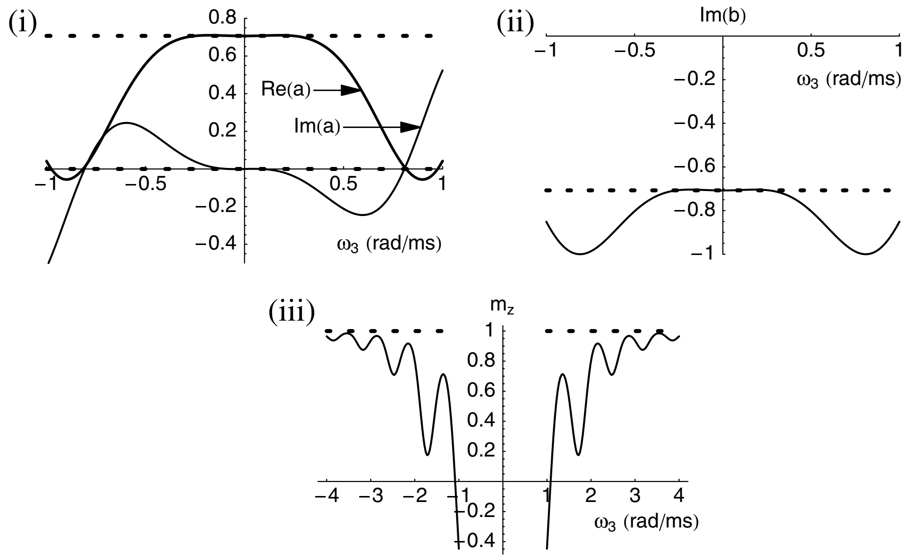

Fig. 3. Response to selective rotation pulse of Fig. 2. (i,ii) The spinor response $s = (a, b)$ in the slice $-1 < \omega_3 < 1$ rad/ms is shown. The real and imaginary parts of a are shown in (i), together with their desired values $[1/\sqrt{2}$ and 0 from Eq. (32)] shown as dashed lines. The imaginary part of b together with its desired value $(-1/\sqrt{2})$ are shown in (ii). The real part of b must be identically zero due to the symmetry of the pulse. (iii) The m_z response outside the slice, assuming initial magnetization $(0, 0, 1)$ is shown. The desired m_z is shown with a dashed line.

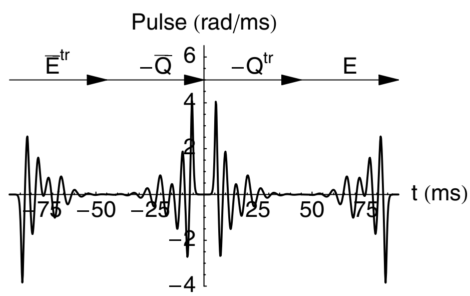

Fig. 4. Selective rotation pulse with $r = 6$ of Example 4.2, designed to produce a $90_x°$ rotation of magnetization within the slice $-1 < \omega_3 < 1$ rad/ms. The individual components of the pulse ($\bar{E}^{tr}$ etc.) are indicated.

half complex plane. This is a good choice, as it results in the pulse with the minimum total energy [19]. This gives, in this case,

$$\Gamma = \frac{1/\sqrt{2}}{\omega_3 + i/\sqrt{2}}. \tag{44}$$

Using the steps described in Section 2.2.2, with $\alpha = 1/\sqrt{2}$, $m = 0$, $n = 1$, and $p_0 = -i/\sqrt{2}$ in Eq. (16), pulse R is

$$R(t) = \frac{2}{\sqrt{2}\cosh t - \sinh t} \quad \text{for } t < 0. \tag{45}$$

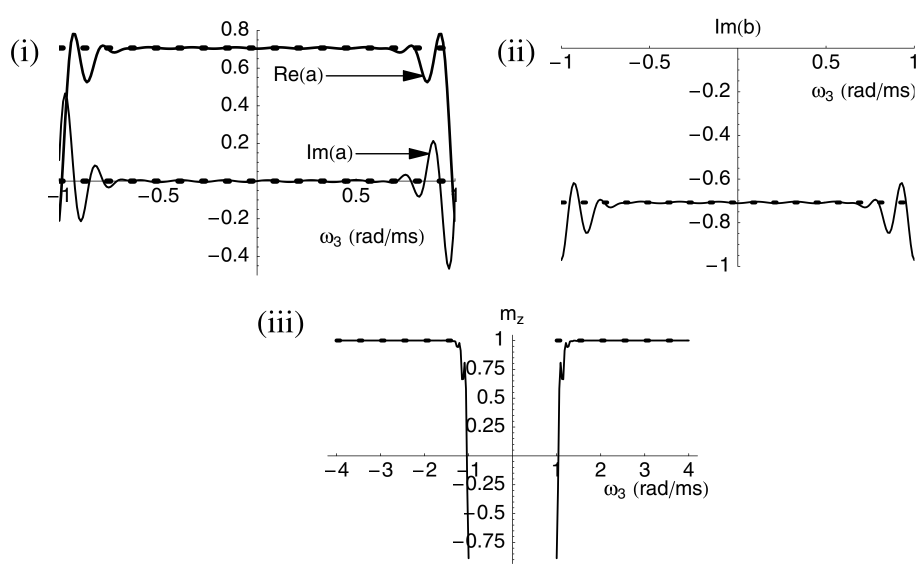

Fig. 5. Spinor response (a, b) inside the slice $-1 < \omega_3 < 1$ rad/ms, and m_z response outside the slice for the selective rotation pulse of Fig. 4. The calculated responses together with the target responses are shown in the same way as in Fig. 3.

Recalling that the refocusing pulse is constructed out of R followed by $R^{\star}(-t)$, then

$$\omega(t) = \frac{2}{\sqrt{2}\cosh|t| + \sinh|t|} \tag{46}$$

is an approximate selective refocusing pulse with

$$b = \frac{-\mathrm{i}}{1+\omega_3^2}. \tag{47}$$

Fig. 6 shows $\omega(t)$ of Eq. (46) and the (numerically calculated) form of the imaginary part of b. Comparing the calculated response to the ideal response for a refocusing pulse, it is clear that most applications would benefit from choosing a larger value of r, as in the next example.

4.4. $180_x°$ selective rotation ($r = 6$)

To find the selective refocusing pulse with response

$$b = \frac{-\mathrm{i}}{1+\omega_3^{12}}. \tag{48}$$

the polynomial equation

$$2|B|^2 + \mathrm{i}\omega_3^6(B - B^{\star}) = 1, \tag{49}$$

where B is a polynomial in ω_3 of order 5, must be solved.

Writing

$$B = B_0 + B_1\omega_3 + B_2\omega_3^2 + \cdots + B_5\omega_3^5, \tag{50}$$

substituting into Eq. (49), and solving the resultant equation for each coefficient of ω_3, 64 possible choices of B can be found. Just as in the previous example, there is a unique choice of B such that $\Gamma = B/(\omega_3^6 + \mathrm{i}B)$ has poles only in the lower half plane (as before, this choice corresponds to the minimum energy pulse). It is (50) with

$$B_0 = \frac{\mathrm{i}}{\sqrt{2}}, B_1 = 2^{5/12}\sqrt{2+\sqrt{3}}, B_2 = -\mathrm{i}2^{1/3}(2+\sqrt{3}),$$
$$B_3 = -\frac{\sqrt{3}}{2^{1/4}}(2+\sqrt{3}), B_4 = \mathrm{i}2^{1/6}(2+\sqrt{3}),$$
$$B_5 = 2^{1/12}\sqrt{2+\sqrt{3}}. \tag{51}$$

In general, for $b = -\mathrm{i}/(1+\omega_3^{2r})$, there are 2^r possible choices of $B = B_0 + B_1\omega_3 + \cdots + B_{r-1}\omega_3^{r-1}$ that satisfy

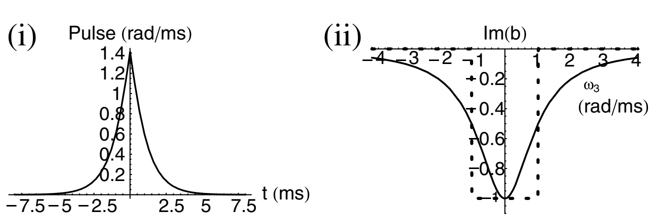

Fig. 6. (i) Selective refocusing pulse, Eq. (46), of Example 4.3, whose spinor response has second component b given by Eq. (47). (ii) Numerically calculated imaginary part of b for this pulse. The ideal form of Im b for a refocusing pulse [from Eq. (26)] is shown as a dashed line. The real part of b must be zero from the symmetry of the pulse.

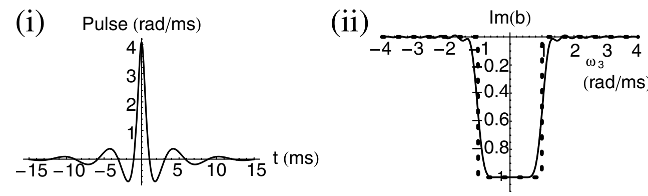

Fig. 7. (i) Selective refocusing pulse of Example 4.4, whose spinor response has second component b given by Eq. (48). (ii) Numerically calculated imaginary part of b for this pulse, with the ideal form of Im b shown as a dashed line.

Eq. (30). There is however only one choice of B such that Γ has poles all in the lower half plane, and this corresponds to the minimum energy pulse (which is purely real).[7] For even (odd) r, $B_0, B_2, \ldots$ are imaginary (real), and $B_1, B_3, \ldots$ are real (imaginary). For $r > 6$, it is difficult to find exact values for the B_j, but they can easily be found numerically.

For the B_j coefficients of (51), Γ was obtained [Eq. (27)], and the algorithm of Section 2.2.2 used to calculate the (real) pulse $R(t)$ for $t < 0$. As in the previous example, the refocusing pulse is then $\omega(t) = R(t)$ for $t < 0$ and $\omega(t) = R^{\star}(-t) = R(-t)$ for $t > 0$.

Fig. 7 shows the refocusing pulse, and the numerically calculated response Im b. As with the $90_x°$ examples, increasing r brings the response close to the ideal response, but at a cost of increased pulse duration and amplitude.

5. Conclusion

Selective rotation pulses can be calculated using inverse scattering methods of pulse design. The desired response is most conveniently specified by a desired spinor response $s_{\mathrm{des}} = (a_{\mathrm{des}}, b_{\mathrm{des}})$ inside the selected frequency band, which is related to the desired flip angle θ and rotation axis (n_x, n_y, n_z) via Eq. (2). It is assumed that outside the selected band, the desired response is that magnetization initially aligned along the z axis [i.e., $m_i = (0, 0, 1)$], will still be aligned along this axis after the pulse [i.e., $m_f = (0, 0, 1)$].

The only constraint on s_{des} is that b_{des} must have a constant phase throughout the slice. Given this constraint, and assuming without loss of generality that b_{des} is purely imaginary, the problem is reduced to finding a selective pulse P with magnetization response Eq. (13), assuming an initial magnetization $(0, 1, 0)$, for all frequency offsets ω_3 in the slice. Finding P can then be reduced to finding pulses Q and E, where these are both standard selective (point to point) pulses, selectively exciting magnetization from $(0, 0, 1)$ to $(0, 1, 0)$ and the (m_x, m_y, m_z) of Eq. (13), respectively.

Section 2.2.2 summarises an algorithm for calculating pulses Q and E, which rely on writing their desired magnetization responses as stereographic projections in rational polynomial form.

[7] These minimum energy pulses can also be found using the inverse scattering method described in [21].

Pulses Q and E can then be used to construct a selective rotation pulse by: (i) truncating each to a duration T (so that each is defined only for $-T < t < 0$), (ii) creating the sequence $E \cdot -Q^{\mathrm{tr}} \cdot -\bar{Q} \cdot \bar{E}^{\mathrm{tr}}$ (where $A \cdot B$ means pulse B followed by pulse A).

Selective refocusing pulses (i.e., when $\theta = 180°$) can be designed using a different procedure that only requires a single sub-pulse, R, to be found. Again, this pulse can be calculated using the method of Section 2.2.2, since it is a standard point to point excitation pulse. The refocusing pulse is then simply $\bar{R}^{\mathrm{tr}} \cdot R$.

Selective rotation pulses can therefore be calculated with response as close as desired to the target response. However, as the accuracy of the rational polynomials used in the calculation of the pulses is increased, so will the pulse duration and amplitude.

How unique these solutions are is currently unknown. For refocusing pulses with desired spinor response described by Eq. (31), there are 2^r possible pulses (but a unique minimum energy pulse). For other values of θ, the situation is less clear. For example, a 0°-selective rotation pulse could be obtained by: (i) using no pulse at all or (ii) the pulse sequence $Q \cdot -Q^{\mathrm{tr}} \cdot -\bar{Q} \cdot \bar{Q}^{\mathrm{tr}}$. A general selective rotation pulse could have a 0°-selective rotation pulse added before or after it without changing its response.

It is not clear whether this is the only source of non-uniqueness for θ-selective rotation pulses, and hence whether the form (14) is always the shortest such pulse (for $\theta \neq 0, \theta \neq \pi$).

References

[1] M.H. Levitt, Composite pulses, Prog. NMR Spectrosc. 18 (1986) 61–122.

[2] J.T. Ngo, P.G. Morris, General solution to the NMR excitation problem for noninteracting spins, Magn. Reson. Med. 5 (1987) 217–237.

[3] H. Geen, R. Freeman, Band-selective radiofrequency pulses, J. Magn. Reson. 93 (1991) 93–141.

[4] L. Emsley, G. Bodenhausen, Optimization of shaped selective pulses for NMR using a quaternion description of their overall propagators, J. Magn. Reson. 97 (1992) 135–148.

[5] J. Shen, Slice-selective J-coupled coherence transfer using symmetric linear phase pulses: applications to localized GABA spectroscopy, J. Magn. Reson. 163 (2003) 73–80.

[6] H.K. Cummins, J.A. Jones, Resonance offset tailored composite pulses, J. Magn. Reson. 148 (2001) 338–342.

[7] I. Roos, K. Mølmer, Quantum computing with an inhomogeneously broadened ensemble of ions: suppression of errors from detuning variations by specially adapted pulses and coherent population trapping, Phys. Rev. A 69 (2004) 022321.

[8] B. Luy, K. Kobzar, T.E. Skinner, N. Khaneja, S.J. Glaser, Construction of universal rotations from point-to-point transformations, J. Magn. Reson. 176 (2005) 179–186.

[9] D.E. Rourke, P.G. Morris, The inverse scattering transform and its use in the exact inversion of the Bloch equation for noninteracting spins, J. Magn. Reson. 99 (1992) 118–138.

[10] J. Schur, Über Potenzreihen, die im Innern des Einheitskreises beschränkt sind, J. Reine Angew. Math. 147 (1917) 205–232.

[11] J. Schur, Über Potenzreihen, die im Innern des Einheitskreises beschränkt sind, J. Reine Angew. Math. 148 (1918) 122–145.

[12] D.E. Rourke, L. Khodarinova, A.A. Karabanov, Two-level systems with relaxation, Phys. Rev. Lett. 92 (2004) 163003.

[13] P. Le Roux, Exact synthesis of radiofrequency waveforms, in: Seventh Annual Meeting and Exhibition, Society of Magnetic Resonance in Medicine, springer, San Francisco, 1988, p. 1049.

[14] M. Shinnar, J.S. Leigh, The application of spinors to pulse synthesis and analysis, Magn. Reson. Med. 12 (1989) 93–98.

[15] S.L. Altmann, Rotations, Quaternions, and Double Groups, Oxford University Press, Oxford, 1986.

[16] J. Pauly, P. Le Roux, D. Nishimura, A. Macovski, Parameter relations for the Shinnar-Le Roux selective excitation pulse design algorithm, IEEE Trans. Med. Imag. 10 (1) (1991) 53–65.

[17] T.P.L. Roberts, T.A. Carpenter, L.D. Hall, A simple method for the construction of 180° refocusing RF pulses for use in nuclear magnetic resonance imaging, J. Magn. Reson. B 101 (1993) 78–82.

[18] W.J. Cody, A survey of practical rational and polynomial approximations of functions, SIAM Rev. 12 (3) (1970) 400–423.

[19] D.E. Rourke, J.K. Saunders, A simple relationship between total RF pulse energy and magnetization response—the nonlinear generalization of Parseval's relation, J. Magn. Reson. A 115 (1995) 189–196.

[20] D.E. Rourke, M.J.W. Prior, P.G. Morris, J.A.B. Lohman, Stereographic projection method of exactly calculating selective pulses, J. Magn. Reson. A 107 (1994) 203–214.

[21] J.W. Carlson, Exact solutions for selective-excitation pulses, J. Magn. Reson. 94 (1991) 376–386.