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Double Swept Band Selective Excitation

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DOUBLESWEPTBANDSELECTIVEEXCITATION

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Double Swept Band Selective Excitation

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Abstract- The paper describes the design of band selective excitation and rotation pulses in high-resolution NMR by the method of double sweep. We first show the design of a pulse sequence that produces band selective excitation to the equator of the Bloch sphere with phase linearly dispersed as frequency. We show how this linear dispersion can then be refocused by nesting free evolution between two adiabatic inversions (sweeps). We then show how this construction can be generalized to give a band selective x rotation over a desired frequency band. Experimental excitation profiles for the residual HDO signal in a sample of 99.5% D_2O are obtained as a function of resonance offset.

I. Introduction

Frequency-selective pulses have widespread use in magnetic resonance and significant effort has been devoted to their design [1]-[46]. Several experiments in high-resolution NMR and magnetic resonance imaging require radiofrequency pulses which excite NMR response over a prescribed frequency range with negligible effects elsewhere. Such band-selective pulses are particularly valuable when the excitation is uniform over desired bandwidth and of constant phase.

In this paper, we propose a new approach for the design of a uniform phase, band selective excitation and rotation pulses. In this approach, using Fourier series, a pulse sequence that produces band selective excitation to the equator of the Bloch sphere with phase linearly dispersed as the frequency is designed. This linear dispersion is then refocused by nesting free evolution between two adiabatic inversions (sweeps). This construction is generalized to give a band selective x-rotation over desired bandwidth. We assume uncoupled spin $\frac{1}{2}$ and neglect relaxation.

Since we use adiabatic sweeps, it should be mentioned that adiabatic sweeps have been previously employed in NMR for producing band selective excitation as in ABSTRUSE pulse sequence [47] and for broadband excitation as in CHORUS [50] and chirp spectroscopy [48, 49].

The paper is organized as follows. In section 2, we present the theory behind double swept **ba**nd**s**elective **e**xcitation, we call **BASE**. In section 3, we present simulation results and experimental data for band selective excitation and rotation pulses designed using double sweep technique. Finally, we conclude in section 4, with discussion and outlook.

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II. Theory

We consider the problem of band selective excitation. Consider the evolution of the Bloch vector X (We use Ω_α to denote the rotation matrix, such that $\alpha \in \{x, y, z\}$) of a spin $\frac{1}{2}$, in a rotating frame, rotating around z-axis at Larmor frequency.

$$\frac{dX}{dt} = (\omega\Omega_z + A(t)\cos\theta(t)\Omega_x + A(t)\sin\theta(t)\Omega_y)X, \quad (1)$$

where $A(t)$ and $\theta(t)$ are amplitude and phase of rf-pulse, and we normalize the chemical shift, $\omega \in [-1, 1]$. In what follows, we choose phase $\sin\theta(t) = 0$ and let

$$\frac{dX}{dt} = (\omega\Omega_z + u(t)\Omega_x)X, \quad (2)$$

where $u(t)$ is the amplitude modulated pulse for $t \in [0, T]$.

Going into the interaction frame of chemical shift, using

$$Y(t) = \exp(-\omega(t - \frac{T}{2})\Omega_z)X(t),$$

we obtain,

$$\frac{dY}{dt} = u(t)(\cos\omega(t - \frac{T}{2})\ \Omega_x - \sin\omega(t - \frac{T}{2})\ \Omega_y)Y;\ Y(0) = \exp(\omega\Omega_z\frac{T}{2})X(0). \quad (3)$$

We design $u(t)$, such that for all $\omega \in [-B, B]$, we have

$$\int_0^T u(t)\cos\omega(t - \frac{T}{2})\ dt \sim \theta, \qquad \int_0^T u(t)\sin\omega(t - \frac{T}{2})\ dt = 0. \quad (4)$$

Divide $[0, T]$ in intervals of step Δt, over which $u(t)$ is constant. Call these amplitudes, $\{u_{-M}, \dots, u_{-k}, \dots, u_0\}$ over $[0, \frac{T}{2}]$ and $\{u_0, \dots, u_k, \dots, u_M\}$ over $[\frac{T}{2}, T]$.

$$\int_0^T u(t)\cos\omega(t - \frac{T}{2})dt \sim (u_0 + \sum_{k=-M}^{M} u_k\cos(\omega k\Delta t))\Delta t, \quad (5)$$

where write $\Delta t = \frac{\pi}{N}$ and choose $u_k = u_{-k}$. This insures that sine equation in Eq. (4) above is automatically satisfied. Then we get,

$$\int_0^T u(t)\cos\omega(t - \frac{T}{2})dt \sim 2\sum_{k=0}^{M} u_k\cos(\omega k\Delta t)\Delta t = 2\sum_{k=0}^{M} u_k\cos(kx)\Delta t, \quad (6)$$

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where for $x \in [-\frac{B\pi}{N}, \frac{B\pi}{N}]$, we have $2\sum_{k=0}^{M} u_k \cos(kx)\Delta t \sim \theta$ and 0 for x outside this range. This is a Fourier series, and we get the Fourier coefficients as,

$$u_0 = \frac{B\theta}{2\pi} \; ; \quad u_k = \frac{2\theta}{\pi}\frac{\sin(\frac{k\pi B}{N})}{\frac{2k\pi}{N}}. \tag{7}$$

For $\theta = \frac{\pi}{2}$, we get,

$$u_0 = \frac{B}{4} \; ; \quad u_k = \frac{\sin(\frac{Bk\pi}{N})}{\frac{2k\pi}{N}}. \tag{8}$$

In Eq. (3), using small flip angle θ, we approximate,

$$Y(T) \sim \exp(\int_0^T u(t)\cos\omega(t-\frac{T}{2})dt\Omega_x)Y(0). \tag{9}$$

Starting from the initial state $X(0) = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$, we have from Eq. 3,

$$X(T) \sim \exp(\frac{\omega T}{2}\Omega_z)\exp(\int_0^T u(t)\cos\omega(t-\frac{T}{2})dt\Omega_x)\exp(\frac{\omega T}{2}\Omega_z)X(0) \sim \exp(\frac{\omega T}{2}\Omega_z)\exp(\frac{\pi}{2}\Omega_x)X(0), \tag{10}$$

for $\omega \in [-B, B]$. There is no excitation outside the desired band.

This state is dephased on the Bloch sphere equator. We show, how using a double adiabatic sweep, we can refocus this phase. Let $\Theta(\omega)$ be the rotation for a adiabatic inversion of a spin. We can use Euler angle decomposition to write,

$$\Theta(\omega) = \exp(\alpha(\omega)\Omega_z)\exp(\pi\Omega_x)\exp(\beta(\omega)\Omega_z). \tag{11}$$

The center rotation should be π, for $\Theta(\omega)$ to do inversion of $\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \rightarrow \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix}$.

We can use this to refocus the forward free evolution. Observe

$$\Delta(\omega, \frac{T}{2}) = \exp(-\frac{\omega T}{2}\Omega_z) = \Theta(\omega)\exp(\frac{\omega T}{2}\Omega_z)\Theta(\omega). \tag{12}$$

Then

$$\Theta(\omega)\ \exp(\frac{\omega T}{2}\Omega_z)\ \Theta(\omega)X(T) \sim \exp(\frac{\pi}{2}\Omega_x)X(0), \tag{13}$$

which is a bandselective excitation.

In summary, the pulse sequence consists of a sequence of x-phase pulses, which produce for $\omega \in [-B, B]$, the evolution

$$U(\omega, \theta) = \exp(\frac{\omega T}{2}\Omega_z)\exp(\theta\Omega_x)\exp(\frac{\omega T}{2}\Omega_z), \tag{14}$$

where $\theta = \frac{\pi}{2}$, as described above, followed by a double sweep rotation $\Delta(\omega, \frac{T}{2})$. This required a peak amplitude of $u(t) \sim \frac{B}{2}$. Fig. 1A shows the pulse sequence for $B = \frac{1}{5}$. The sweep(chirp) is done with a peak amplitude of $\frac{1}{2}$, $T = 40\pi$.

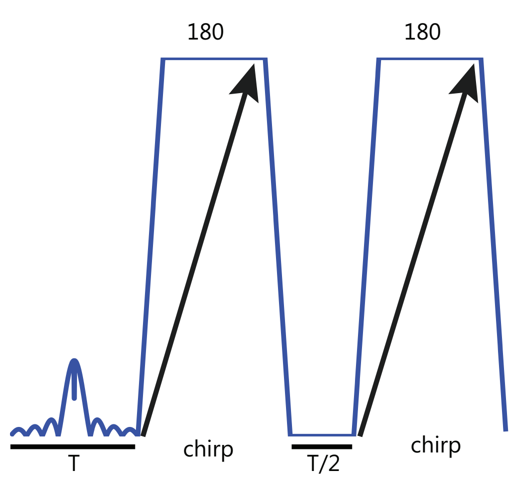
We talked about band selective excitations. Now we discuss band selective $\frac{\pi}{2}$ rotations. This is simply obtained from above by an initial double sweep. Thus

$$U_1 = \Delta(\omega, \frac{T}{2})\ U(\omega, \frac{\pi}{2})\ \Delta(\omega, \frac{T}{2}), \tag{15}$$

is a $\frac{\pi}{2}$ rotation around the x-axis. Fig. 1B shows the band selective rotation pulse sequence for $B = .2$. The chirp is done with a peak amplitude of $\frac{1}{2}$, $T = 40\pi$.

If there is rf-inhomogeneity, then Eq. (2) takes the form $\frac{dX}{dt} = (\omega\Omega_z + \epsilon u(t)\Omega_x)X$, where ϵ is inhomogeneity parameter which takes value 1 in the ideal case. The evolution in Eq. (10) then takes the form $X(T) \sim \exp(\frac{\omega T}{2}\Omega_z)\exp(\epsilon\frac{\pi}{2}\Omega_x)X(0)$. The excitation angle is therefore linearly effected by rf-inhomogeneity.

A



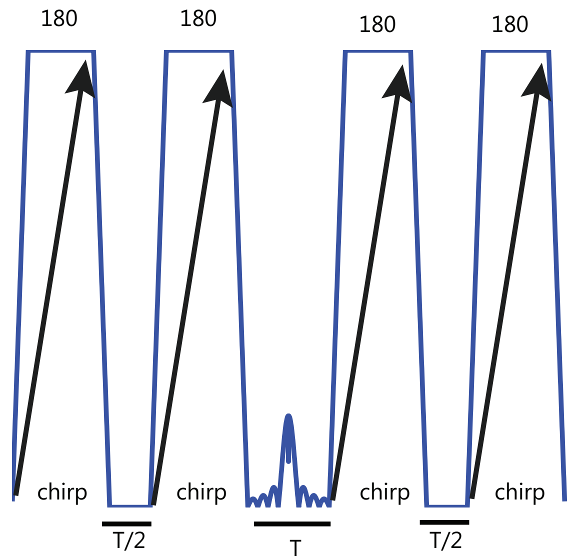


Figure 1: Fig. A, shows the **BASE** pulse sequence (amplitude) with a double sweep that performs band selective excitation as in Eq. (13) for $B = \frac{1}{5}$. Fig. B, shows the **BASE** pulse sequence with two double sweeps that performs band selective rotation as in Eq. (15) for $B = \frac{1}{5}$.

III. Simulations

We normalize ω in Eq. (1), to take values in the range $[-1, 1]$. We choose time $\frac{T}{2} = M\pi$, where we choose $M = 20$ and $N = 10$ in $\Delta t = \frac{\pi}{N}$ in Eq. (5). Choosing $\theta = \frac{\pi}{2}$ and coefficients u_k as in Eq. (8), we get the value of the Eq. (6) as a function of bandwidth as shown in left panel of Fig. 2 for $B = .2$. This is a decent approximation to $\frac{\pi}{2}$ over the desired bandwidth. The right panel of Fig. 2, shows

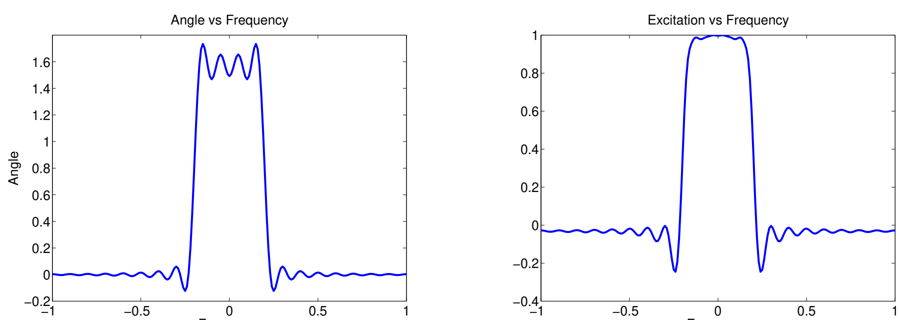


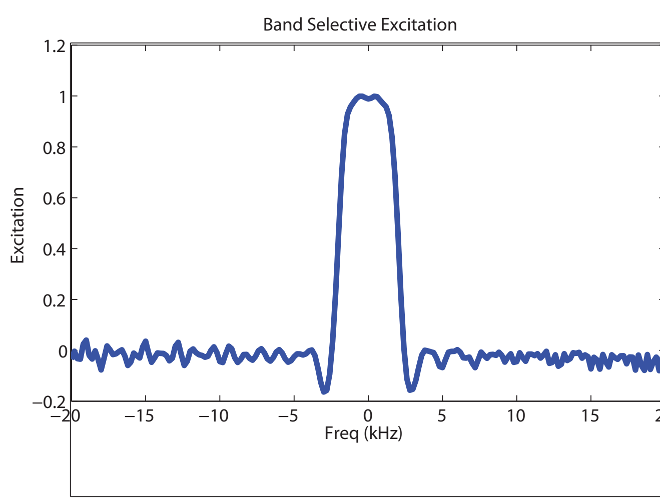
Figure 2: Left panel shows the value of the Eq. (6) as a function of bandwidth when we choose $T = 40\pi$ and $\Delta t = \frac{\pi}{10}$, $B = \frac{1}{5}$. The right panel shows the excitation profile i.e., the $-y$ coordinate of the Bloch vector, after application of the pulse in Eq. (13), with u_k

the excitation profile i.e., the $-y$ coordinate of the Bloch vector after application of the pulse in Eq. (13), where we assume that adiabatic inversion is ideal. The peak rf-amplitude $A \sim \frac{B}{2}$ for $B = .2$.

Next, we implement the nonideal adiabatic sweep with a chirp pulse, by sweeping from $[-1.5, 1.5]$ in 300 units of time. This gives a sweep rate $\frac{1}{100} \ll A^2$, where $A = \frac{1}{2}$. The chirp pulse is a depicted in Fig. 1. The chirp operates at its peak amplitude over sweep from $[-1, 1]$. The resulting excitation profile of Eq. (13) is shown in Fig. 3 A, where we show the $-y$ coordinate of the Bloch vector. After scaling, $\omega \in [-20, 20]$ kHz, $B = 2$ kHz and $A = 10$ kHz, this pulse takes 6.27 ms. In Fig. 3 B, and 3 C, we have $B = 4$ kHz and $B = 8$ kHz respectively. The pulse time is same 6.27 ms. $T = 1$ ms in Fig. 1A.

Next, we simulate the band selective x rotation as in Eq. (15). This requires to perform double sweep twice as in Eq. (15). Adiabatic sweep is performed as before. The resulting excitation profile of Eq. (15) is shown in Fig. 4 A,B and C, where we show the z coordinate of the Bloch vector starting from initial $y = 1$ for $B = [-2, 2]$ kHz, $B = [-4, 4]$ kHz and $B = [-8, 8]$ kHz respectively. This pulse takes 11.54 ms in each case.

A



B

C

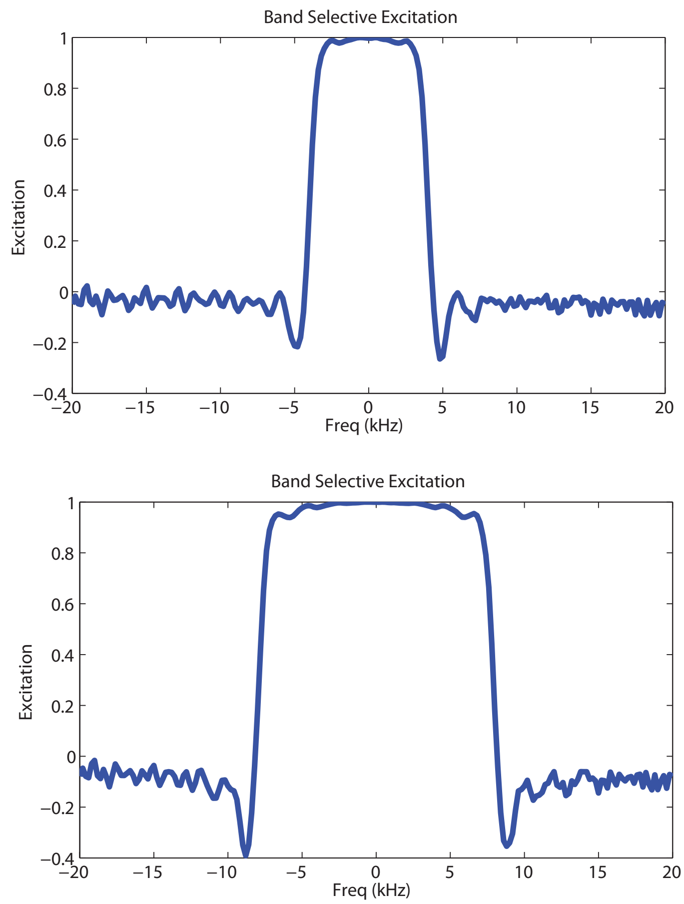
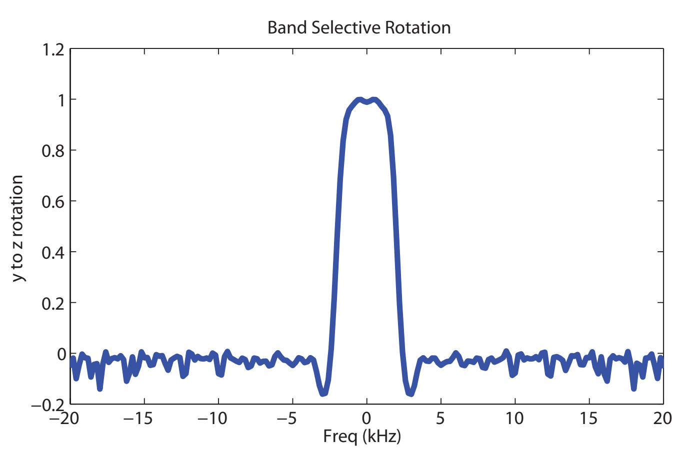


Figure 3: Fig. A, B, C shows the excitation profile (the $-y$ coordinate of Bloch vector) for the **BASE** pulse in Eq. (13) with $B = [-2, 2]$ kHz, $B = [-4, 4]$ kHz and $B = [-8, 8]$ kHz, respectively. The peak amplitude is $A = 10$ kHz. Time of the pulse is 6.27 ms. $T = 1$ ms in Fig. 1A.

a) Experimental

All experiments were performed on a 750 MHz (proton frequency) NMR spectrometer at 298 K. Fig. 5 shows the experimental excitation profiles for the residual HDO signal

A



C

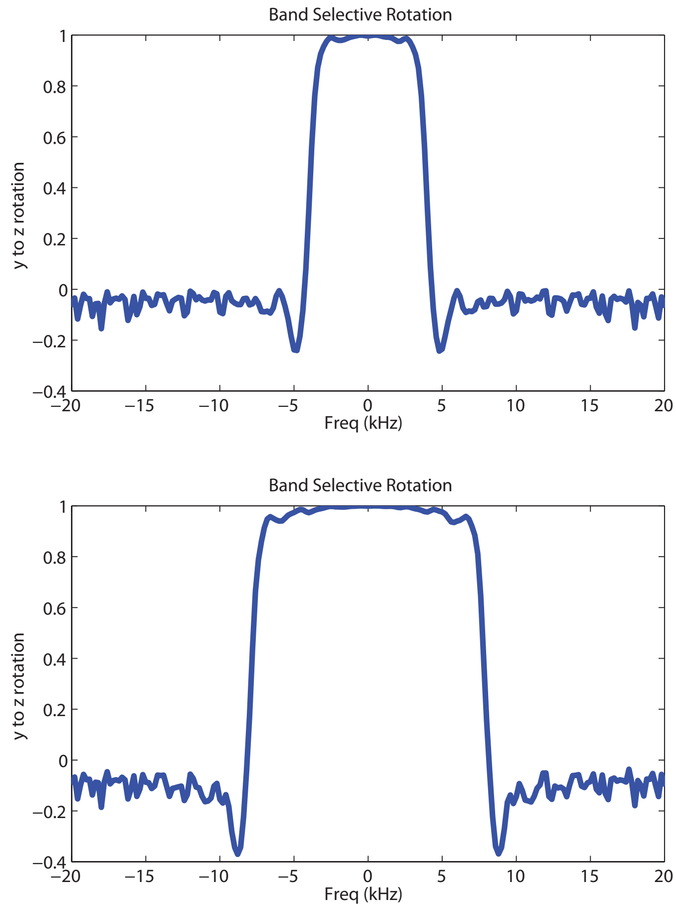


Figure 4: Fig. A, B, C shows the y to z rotation profile (the z coordinate of Bloch vector) for the band selective x rotation pulse in Eq. (15) with $B = [-2, 2]$ kHz, $B = [-4, 4]$ kHz and $B = [-8, 8]$ kHz, respectively. The peak amplitude is $A = 10$ kHz. Time of the pulse is 11.54 ms. $T = 1$ ms in Fig. 1B.

in a sample of 99.5% D_2O displayed as a function of resonance offset. Fig. 5A, B, C shows the excitation profile of **BASE** sequence in Fig. 3 A, B, C respectively. The frequency band of interest is $[-2, 2]$ kHz, $[-4, 4]$ kHz and $[-8, 8]$ kHz respectively. In each case, the peak amplitude of the rf-field is 10 kHz and duration of the pulse is 6.27 ms. The pulse sequence uses one double sweep. $T = 1$ ms in Fig. 1A. To show the performance of the **BASE** sequence as a function of frequency, the offset is varied over a range of [-20, 20] kHz with on-resonance at 3.53 kHz (4.71 ppm).

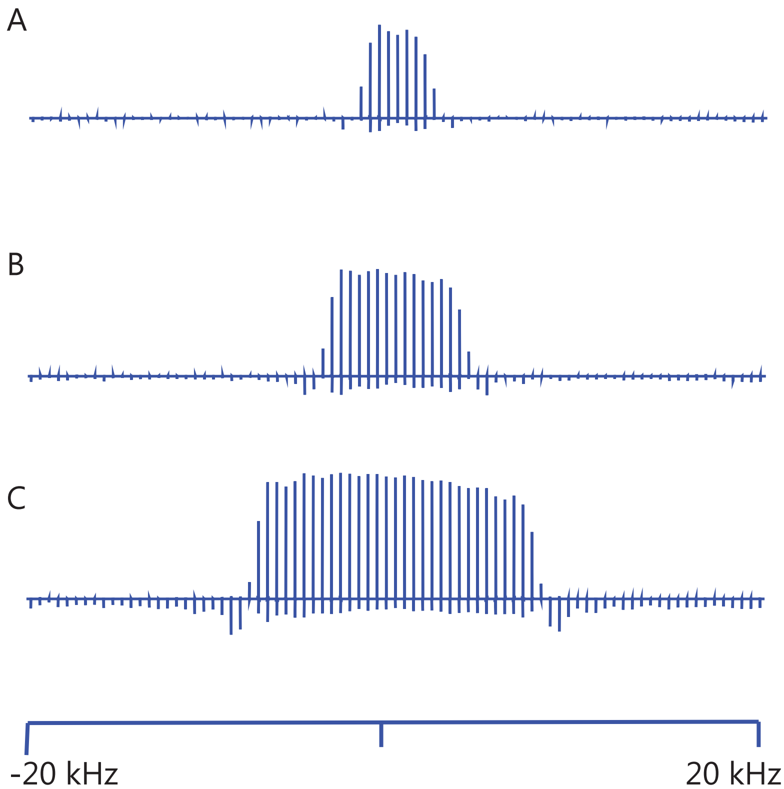
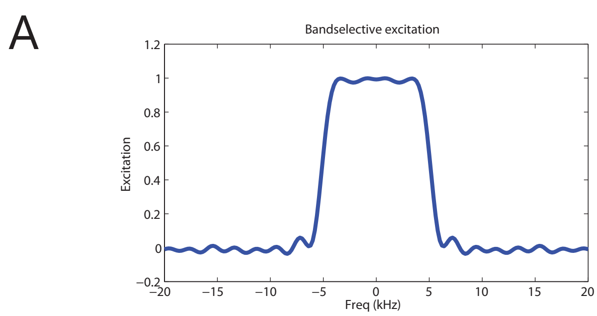


Figure 5: Fig. A, B, C show the experimental excitation profile of **BASE** sequences in Fig. 3A,B and C, respectively, with $B = [-2, 2]$ kHz, $B = [-4, 4]$ kHz and $B = [-8, 8]$ kHz, respectively, in a sample of 99.5% D_2O. The offset is varied over the range as shown and the peak rf power of all pulses is 10 kHz. The duration of the pulses is 6.27 ms.

IV. Conclusion

In this paper we showed design of band selective excitation and rotation pulses (**BASE**). We first showed how by use of Fourier series, we can design a pulse that



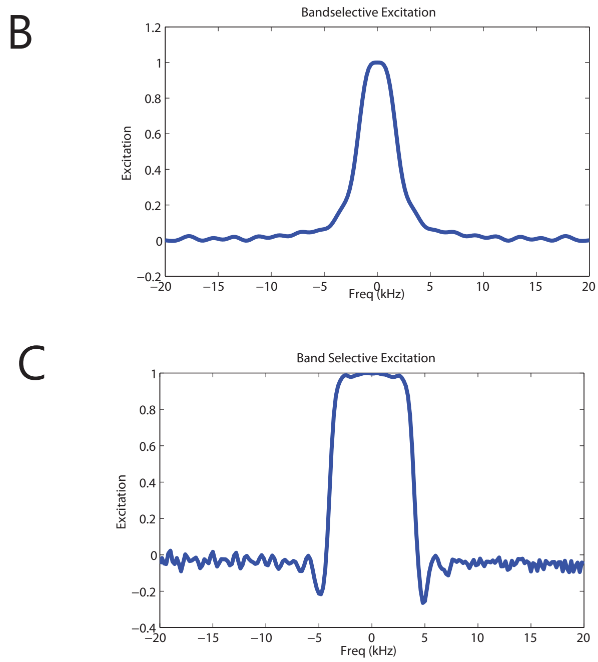


Figure 6: Fig. A, B, C show the simulations of excitation profile of **BURP**, **SNOB** and **BASE** sequences respectively. The excitation bandwidth of **BURP** sequence is $[-4, 4]$ kHz and is .5 ms sequence. The excitation bandwidth of **SNOB** sequence is $[-2.8, 2.8]$ kHz and is .5 ms sequence. The excitation bandwidth of **BASE** sequence is $[-4, 4]$ kHz and is 6.27 ms sequence.

does band selective excitation to the equator of Bloch sphere. The phase of excitation is linearly dispersed as function of offset, which is refocused by nesting free evolution between adiabatic inversion pulses. We then extended the method to produce band selective rotations. The pulse duration of the pulse sequences is largely limited by time of adiabatic sweeps. This increases, if we have larger working bandwidth. However, for very large bandwidths, we may invert only the band of interest. Thereby, we may be able to reduce the time of the proposed pulse sequences.

It is worthwhile, to compare the **BASE** sequence, with state of the art pulse sequences like **BURP** [22] and **SNOB** [32]. In **BURP** and **SNOB**, the pulse sequence is amplitude modulated, with amplitude $u(t)$, parameterized through a Fourier series as,

$$u(t) = \frac{2\pi}{T}(a_0 + \sum_{k=1}^{n} a_k \cos\frac{2\pi kt}{T} + b_k \sin\frac{2\pi kt}{T}),$$

where T is pulse duration and the Fourier coefficients a_k, b_k are determined by a simulated annealing optimization procedure [22]. Fig. 6 shows the simulations of excitation profile of **BURP**, **SNOB** and **BASE** sequences. The transition from passband to stopband is much sharper for the **BASE** sequence. Although Fourier series appears in all these sequences, its manifestation in **BASE** is very different from **BURP** and **SNOB**, making it possible to analytically design rather than numerically optimize.

The principle merit of the proposed **BASE** pulse sequence is the analytical tractability and conceptual simplicity of the design.

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