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

Index terms—

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

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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 2 O are obtained as a function of resonance offset.

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 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 AB-STRUSE 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 bandselective excitation, 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.

2 Introduction

We consider the problem of band selective excitation. Consider the evolution of the Bloch vector X (We use ? ? to denote the rotation matrix, such that ? ? {x, y, z}) of a spin 1 2 , in a rotating frame, rotating around z-axis at Larmor frequency.dX dt = (?? z + A(t) cos ?(t)? x + A(t) sin ?(t)? y)X,**(1)**

II.

3 Theory

where A(t) and ?(t) are amplitude and phase of rf-pulse, and we normalize the chem-ical shift, ? ? [?1, 1].

In what follows, we choose phase sin ?(t) = 0 and letdX dt = (?? z + u(t)? x)X,**(2)**

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

Going into the interaction frame of chemical shift, usingY (t) = exp(??(t ? T 2)? z)X(t),

we obtain,dY dt = u(t)(cos ?(t ? T 2) ? x ? sin ?(t ? T 2) ? y)Y ; Y (0) = exp(?? z T 2)X(0). (**3**)

We design u(t), such that for all ? ? [?B, B], we haveT 0 u(t) cos ?(t ? T 2) dt ? ?, T 0 u(t) sin ?(t ? T 2) dt = 0.**(4)**

Divide [0, T] in intervals of step ?t, over which u(t) is constant. Call these amplitudes, {u ?M , . . . , u ?k , . . . , u 0 } over [0, T 2] and {u 0 , . . . , u k , . . . , uM } over [T 2 , T]. T 0 u(t) cos ?(t ? T 2)dt ? (u 0 + M k=?M u k cos(?k?t))?t,**(5)**

where write ?t = ? N and choose u k = u ?k . This insures that sine equation in Eq. (4) above is automatically satisfied. Then we get, where for x ? [? B? N , B? N], we have 2 M k=0 u k cos(kx)?t ? ? and 0 for x outside this range. This is a Fourier series, and we get the Fourier coefficients as,T 0 u(t) cos ?(t ? T 2)dt ? 2 M k=0 u k cos(?k?t)?t = 2 M k=0 u k cos(kx)?t,**(6)**u 0 = B? 2? ; u k = 2? ? sin(k?B N) 2k? N .**(7)**

For ? = ? 2 , we get,u 0 = B 4 ; u k = sin(Bk? N) 2k? N .**(8)**

In Eq. (3), using small flip angle ?, we approximate,Y (T) ? exp(T 0 u(t) cos ?(t ? T 2)dt? x)Y (0). (**9**)

Starting from the initial stateX(0) = ? ? 0 0 1 ? ? , we have from Eq. 3, X(T) ? exp(?T 2 ? z) exp(T 0 u(t) cos ?(t? T 2)dt? x) exp(?T 2 ? z)X(0) ? exp(?T 2 ? z) exp(? 2 ? x)X(0),**(10)**

for ? ? [?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 ?(?) be the rotation for a adiabatic inversion of a spin. We can use Euler angle decomposition to write,?(?) = exp(?(?)? z) exp(?? x) exp(?(?)? z). (**11**)

The center rotation should be ?, for ?(?) to do inversion of? ? 0 0 1 ? ? ? ? ? 0 0 ?1 ? ? .

We can use this to refocus the forward free evolution. Observe ?(?, T 2) = exp(? ?T 2 ? z) = ?(?) exp(?T 2 ? z)?(?). (**12**)F Then ?(?) exp(?T 2 ? z) ?(?)X(T) ? exp(? 2 ? x)X(0),**(13)**

which is a bandselective excitation.

In summary, the pulse sequence consists of a sequence of x-phase pulses, which produce for ? ? [?B, B], the evolutionU (?, ?) = exp(?T 2 ? z) exp(?? x) exp(?T 2 ? z),**(14)**

where ? = ? 2 , as described above, followed by a double sweep rotation ?(?, T 2). This required a peak amplitude of u(t) ? B 2 . Fig. 1A shows the pulse sequence for B = 1 5 . The sweep(chirp) is done with a peak amplitude of 1 2 , T = 40?.

We talked about band selective excitations. Now we discuss band selective ? 2 rotations. This is simply obtained from above by an initial double sweep. ThusU 1 = ?(?, T 2) U (?, ? 2) ?(?, T 2),**(15)**

is a ? 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 1 2 , T = 40?.

If there is rf-inhomogeneity, then Eq. (2) takes the form dX dt = (?? z + ?u(t)? x)X, where ? is inhomogeneity parameter which takes value 1 in the ideal case. The evolution in Eq. (10) then takes the form X(T) ? exp(?T 2 ? z) exp(? ? 2 ? x)X(0). The excitation angle is therefore linearly effected by rf-inhomogeneity. 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 ? 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 1 100 ? A 2 , where A = 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, ? ? [?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 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 IV. 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.

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It is worthwhile, to compare the BASE sequence, with state of the art pulse se-Double Swept Band Selective Excitation quences like BURP [22] and SNOB [32]. In BURP and SNOB, the pulse sequence is amplitude modulated, with amplitude u(t), parameterized through a Fourier 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. [1]

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