RF pulse design for adiabatic spin decoupling

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Introduction

Spin decoupling is a standard technique in in-vitro NMR to simplify spectra and for signal enhancement. The application in-vivo, however, is much more sophisticated because of specific SAR and hardware limitations. Adiabatic pulses can achieve spin inversion over very large bandwidths which favors their use as basic building blocks of decoupling sequences in high-resolution NMR at highest Zeeman fields [1]. For MRI applications the low peak RF amplitude and efficient use of energy over the bandwidth as well as the relative insensitivity to RF inhomogeneities may be the most important advantages of adiabatic pulses. The paper presents the design and application of an adiabatic pulse specifically for spin decoupling in-vivo at high field.

Methods

We consider ^{1}H decoupling, as applied, e.g. in carbon and phosphorous MRS, on a high-field scanner of 3 to 4T field strength. The chemical shift range of hydrogen is then of the order of 1200 to 1600 Hz (10ppm). To achieve admissible SAR, the pulse amplitude should be as small as possible. However, a certain RF field strength is necessary to maintain adiabaticity throughout the pulse. Also, decoupling side bands get stronger as their intensity is inversely proportional to the square of the RF amplitude [2]. Further on, the pulse length should not exceed the reciprocal of the scalar coupling strength (e.g. 120 to 140 Hz for 1-bond ^{1}H – ^{13}C couplings) because phase cycling schemes compensating imperfections of the decoupling sequence become to long to operate properly and because side bands accumulate more densely [2]. To match these specifications we settle with the design of an adiabatic pulse of length 4 ms, operating over a bandwidth of 1600 Hz at possibly small peak amplitude, still achieving excellent adiabatic spin inversion. Recently, a method was proposed which allows within a family of pulse shapes the trade-off between duration τ, bandwidth σ, peak amplitude ω, transition width δ, and adiabaticity parameter k [3]. The pulses are characterized by a linear frequency sweep at constant RF amplitude and a specific apodization to begin and terminate the pulse smoothly (an elliptical path of the effective field). The start configuration τ = 9 ms, σ = 7.27 kHz, ω = 770 Hz, δ = 760 Hz, and k = 3 determines an excellent adiabatic inversion pulse [3]. In intermediate steps, the amplitude is firstly reduced to 570 Hz by setting the bandwidth and length to the desired values of 1.6 kHz and 4 ms, respectively. Secondly, a further reduction is achieved by increasing the transition width to 6 kHz (also k had to be raised to 8.3 to obey adiabatic following). The width of the transition region inverted/non-inverted magnetization is of no relevance to the decoupling problem because the resonances of all hydrogen nuclei are covered by the inversion bandwidth. The normalized shape of the pulse finally obtained and to be used for decoupling is shown in Fig. 1. A simulation of the inversion performance by contours of longitudinal magnetization at the end of the pulse (normalized with respect to the initial equilibrium magnetization) in dependence of resonance offset and peak RF amplitude is presented in Fig. 2. The pulse achieves reasonably good inversion over a bandwidth of 1.6 kHz at peak amplitude 400 Hz and is insensitive to RF variations in the range 400 to over 1100 Hz. For comparison, the inversion profile of the well-known hyperbolic secant adiabatic pulse (HS) of equal bandwidth and duration is also presented [4]. The decoupling sequence consists of a windowless repetition of the new adiabatic inversion pulse with a phase cycle to compensate for imperfections [2]. The 5-step cycle $(0^{o},150^{o},60^{o},150^{o},0^{o})$ nested within the 4-step cycle MLEV-4 $(0^{o},0^{o},180^{o},180^{o})$ is used, since this has been shown to give best results when adiabatic pulses are used as basic building blocks [1]. Experiments are performed on a standard 600 MHz high-resolution NMR spectrometer, equipped with a triple resonance probe, on a sample of Menthol (500 µl of 30 vol-% of Menthol with naturally abundant ^{13}C in deuterated Chloroform). A non-selective RF pulse is used for carbon excitation. Subsequently, 32 scans of 16384 data points sampled during ^{1}H decoupling at 31.5 µs dwell time are co-added. Zero-filling to 32768 data points but no filtering is applied prior to Fourier transformation. Only the most down-field shifted signal, the carbonyl carbon, is considered. For determination of the decoupling bandwidth, the carrier frequency of the decoupling RF field is set to the Larmor frequency of the directly bound ^{1}H and varied to offsets +/– 1400 Hz in steps of 200 Hz. The scalar coupling between the carbonyl carbon and the directly bound hydrogen is ~140 Hz.

Results and Discussion

In Fig. 3, the carbonyl carbon line is shown in dependence of the decoupler offset to the directly bond hydrogen. The decoupling sequence has a peak RF amplitude of only 400 Hz and a RMS amplitude of 370 Hz. Proper decoupling occurs over a bandwidth of ~1600 Hz. Cycling sidebands are, depending on resonance offset, of the order of 5% to 15% of the central line. In comparison (data not shown), adiabatic decoupling of similar quality based on the HS pulse requires peak and RMS RF amplitude of 870 Hz and 375 Hz, respectively, with sidebands increased by ~ 10%. The side bands are unusually strong because of the unprecedented low decoupler amplitude. They can be largely eliminated by asynchronous detection and phase permutation [2] which are not applied in the current experiments. Adiabatic spin decoupling based on the newly designed pulse obeys the principle requirements for in-vivo application at high field: broadband performance at sufficiently low power and peak RF amplitude. Dedicated applications, like the acquisition of decoupled spectra using surface coils may become feasible because adiabatic decoupling is rather insensitive to RF inhomogeneity. Suitable pulses can be designed along similar lines with the aim to extend in-vivo adiabatic spin decoupling to ultra-high fields.

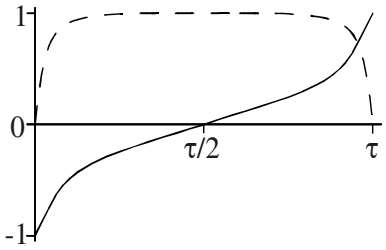

Fig. 1: Normalized amplitude (dashed) and frequency (solid) modulation of the new pulse (length τ) vs. time.

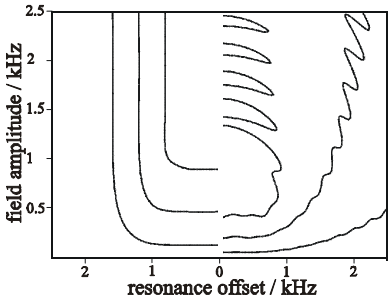

Fig. 2: Calculated normalized longitudinal magnetization at the end of new pulse (RHS) and HS (LHS). Contours are -0.9 (inner), 0 (middle), and 0.9 (outer)..

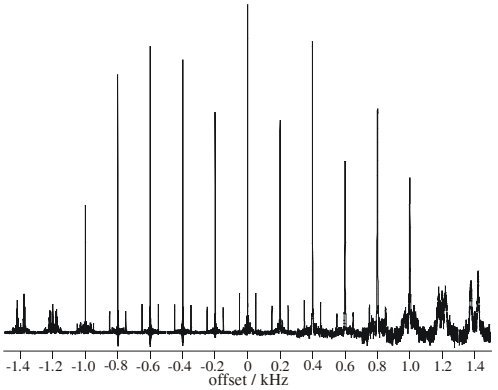

Fig. 3: Carbonyl carbon line of Menthol in dependence of offset of decoupling field of amplitude 400 Hz to Larmor frequency of directly bound hydrogen (J ~ 140 Hz).

References

[1] De Graaf R. A., Magn Reson Med **53**, 1297 (2005). [2] Shaka A. J., et al. Prog. Nucl. Magn. Reson. Spectrosc. **19**, 47 (1987). [3] Mitschang L., Magn. Reson. Med. **53**, 1217 (2005). [4] Silver M. S., et al., Phys. Rev. A **31**, 2753 (1985).