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Short Perspective on "NMR Population Inversion Using a Composite Pulse" by M.H. Levitt and R. Freeman [J. Magn. Reson. 33 (1979) 473–476]

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ABSTRACT

Article history: Available online 7 September 2011 The invention of the composite pulse by Malcolm H. Levitt in 1978 is described from a personal perspective. © 2011 Elsevier Inc. All rights reserved.

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Interview with the author(s).

A video interview with the author(s) associated with this Historical Perspective and the original article can be found in the online version, at doi:10.1016/j.jmr.2011.08.016.

In 1978 I was a 4th year undergraduate studying Chemistry at Oxford University. The undergraduate degree came in two parts: Part 1 was the usual lecture-based course, assessed by tough final examinations at the end of the 3rd year. Part 2 was an experimental project based in a research laboratory. As an undergraduate I was particularly inspired by the wonderful quantum mechanics lectures of Peter Atkins, and I wanted to research on something to do with quantum mechanics. Atkins could not take me on that year so I went for my second choice supervisor, who was Ray Freeman. Although his lectures were very entertaining they were almost lacking in theory – nevertheless I felt that NMR probably had something to do with quantum mechanics, and it turned out that I was not disappointed.

In Ray Freeman's lab I was inducted into the subject by Geoffrey Bodenhausen, who was just leaving the laboratory having completed his doctorate. Geoffrey taught me how to program the spectrometer (using octal machine code) and how to use magnetization vectors to understand NMR. I was assigned a project concerned with spin echoes (the details of which I have forgotten). The experiments never worked well, and I learnt from Geoffrey that this was probably due to radiofrequency inhomogeneity, which was quite severe on our instrument (an antiquated Varian CFT-20 equipped with a water-cooled electromagnet).

I had studied the spin echo phenomena of Hahn [1], Carr and Purcell [2], and enjoyed how the spreading of the magnetization vectors under the action of static field inhomogeneity could be reversed by applying a 180 degree pulse. Could a similar thing be done for radiofrequency field inhomogeneity? If I could figure that out, I might be able to complete my project anyway. I learnt about the rotary echoes of Solomon [3] in which the spreading effect of radiofrequency field inhomogeneity is reversed by a 180 degree phase shift. Although the phenomenon of rotary echoes demonstrates that radiofrequency field inhomogeneity may indeed be reversed, the effect is not very useful, since the net rotation generated by a rotary echo is always zero. Was it possible to compensate radiofrequency field inhomogeneity, while still imposing a net rotation on the nuclei? That seemed unlikely, but it was worth thinking about.

It occurred to me that the vector picture used to explain the formation of spin echoes could be tipped on its side to predict a refocussing effect for radiofrequency inhomogeneity, while still generating a net 180-degree rotation of the nuclear spins (see accompanying video). This reasoning suggested a sequence of three pulses with different phases: $90_x 180_y 90_x$. The two outer 90 degree pulses would be subject to errors caused by radiofrequency field inhomogeneity, but the central 180 degree pulse would exchange the positions of the magnetization vectors, just as in a spin echo, causing the errors in the outer rotations to compensate each other. Although this would not work perfectly since the central 180 degree pulse was also imperfect, I reasoned that for small imperfections the error in the central pulse would not matter too much since the vectors did not have to rotate far. I knew just enough mathematics to work out the equations and my hunch seemed to be correct. The sequence of three pulses generated a more accurate inversion





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of z-magnetization than a single pulse, in the presence of a small amount of radiofrequency inhomogeneity. I had a self-compensating sequence of pulses!

At that time there was a blue notebook on the windowsill in Ray Freeman's lab, in which members of the group were encouraged to sketch down any ideas they had, however absurd. I hope that the book still exists since many ideas that turned out to be important first appeared there, such as several different forms of two-dimensional spectroscopy, as well as the classic DANTE [4], INEPT [5] and INADEQUATE sequences [6] (as well as many completely loopy ideas that are better left hidden). I wrote up my first ever research idea on a single page of the "blue book" (see accompanying video) and showed it to Gareth Morris. Somewhat to my surprise Gareth thought the idea was original and we went off to have tea and cakes to celebrate. The idea was very much to Ray's taste and he coined the elegant term "composite pulse". This was based. I believe, on the mechanics of accurate watches, where strips of metals with different thermal expansion coefficients are bonded together so that the composite metallic strip is compensated against changes in temperature.

I was dispatched to write FORTRAN code for a miraculous new ink plotter that had been installed at the central computer laboratory. Gareth had already generated plots for his DANTE sequence [4] so I simply had to adapt his code and go through the laborious process of punching a stack of cards, feeding them into the infernal machine, and waiting overnight for the plot to be delivered. The results were very beautiful and appeared in the 1979 publication.

It turned out that I had struck gold with my very first stroke of the spade. Magnetic resonance theory is full of rotations, so an idea that shows some novel properties of rotations has a lot of mileage. Later on, I would apply these ideas to the problem of efficient heteronuclear decoupling [7], and eventually to pulse sequence design in solid-state NMR as well [8–10]. For many years I would learn about whole areas of magnetic resonance by working out possible applications of composite pulses. In retrospect, the composite pulse is one of those simple, almost naive, ideas that conceals hidden depths. The field of "quantum control" studies the manipulation of quantum mechanical systems by sets of "control fields". A particularly important problem in quantum control is how to achieve "quantum error correction" [11]. In the context of NMR, these advanced concepts have led to sophisticated "optimum control" modulation schemes, which are far more effective than composite pulses [12]. Nevertheless, the composite pulse demonstrates the principles of "quantum error correction" in such a simple way that almost anyone can visualise and appreciate it – and indeed, almost anyone could have invented it!

References

- [1] E.L. Hahn, Spin echoes, Phys. Rev. 80 (1950) 580-594.
- [2] H.Y. Carr, E.M. Purcell, Effects of diffusion on free precession in nuclear magnetic resonance experiments, Phys. Rev. 94 (1954) 630–638.
- [3] I. Solomon, Rotary spin echoes, Phys. Rev. Lett. 2 (1959) 301-302.
- [4] G.A. Morris, R. Freeman, Selective excitation in Fourier transform nuclear magnetic resonance, J. Magn. Reson. 29 (1978) 433-462.
- [5] G.A. Morris, R. Freeman, Enhancement of nuclear magnetic resonance signals by polarization transfer, J. Am. Chem. Soc. 101 (1979) 760–762.
- [6] A. Bax, R. Freeman, S.P. Kempsell, Natural abundance 13C–13C coupling observed via double-quantum coherence, J. Am. Chem. Soc. 102 (1980) 4849– 4851.
- [7] M.H. Levitt, R. Freeman, Composite pulse decoupling, J. Magn. Reson. 43 (1981) 502.
- [8] M.H. Levitt, D. Suter, R.R. Ernst, Composite pulse excitation in three-level systems, J. Chem. Phys. 80 (1984) 3064.
- [9] Y.K. Lee, N.D. Kurur, M. Helmle, O.G. Johannessen, N.C. Nielsen, M.H. Levitt, Efficient dipolar recoupling in the NMR of rotating solids: a seven-fold symmetric radiofrequency pulse sequence, Chem. Phys. Lett. 242 (1995) 304– 309.
- [10] M. Hohwy, H.J. Jakobsen, M. Edén, M.H. Levitt, N.C. Nielsen, Broadband dipolar recoupling in the NMR of rotating solids: a compensated C7 pulse sequence, J. Chem. Phys. 108 (1998) 2686.
- [11] E. Knill, R. Laflamme, W.H. Zurek, Resilient quantum computation, Science 279 (1998) 342–345.
- [12] N. Khaneja, R. Brockett, S.J. Glaser, Time optimal control in spin systems, Phys. Rev. A 63 (2001).