Implementing Optimal Control Pulses in ESR using an Arbitrary Microwave Waveform Generator

D.L. Goodwin, W.K. Myers, C.R. Timmel, and I. Kuprov

1 School of Chemistry, University of Southampton, Highfield Campus, Southampton SO17 1BJ, United Kingdom,
2 Department of Chemistry, Centre for Advanced Electron Spin Resonance, University of Oxford, South Parks Road, Oxford OX1 3QR, United Kingdom

Microwave pulses with variable amplitude and phase can be designed, using optimal control theory, to achieve higher excitation bandwidth, and hence higher sensitivity, than hard pulses. The main problems in directly applying optimal control techniques [1] (designed originally for NMR) to EPR spectroscopy are the time-scales and the spectral widths involved.

Bruker SpinJet, an arbitrary waveform generator (AWG), makes it possible to use a discretised pulse shape to realise those optimal control solutions. However, waveforms produced by an AWG inevitably become distorted in transit between the AWG and the sample. A number of solutions have been proposed for creating a transfer matrix to transform the proposed input waveform to that seen by the sample [2, 3, 4].

In this communication we propose forming a transfer matrix from measurements at the transmission monitor, after the AWG. This transfer matrix is then used within a cost function for quasi-Newton optimisation (tolerant to static noise), then simulated with gradient ascent pulse engineering (GRAPE) [1]. Typical optimal control pulses involve sharp transients and it is expected that those would generate pronounced waveform distortions. To reduce this effect, we propose the use of smoothing Tikhonov regularisation functions within the optimisation.

The numerical solutions produced by the cost functional cost functional described above would not be optimal in the strict sense; further waveform distortions are expected to be sample- and resonator-specific. The proposition here is to use the GRAPE solution as a starting point, close enough to a local minimiser, from which a modified simplex method, running in a direct measurement feedback loop on an actual instrument, would not struggle to find a minimiser proper.

This work is supported by funding from QUAINT EU FP7, EPSRC iMR-CDT, and EPSRC grant to Centre for Advanced Spin Resonance EP/L011972/1.


