

ihMT, MLBS and SIMPSON

A tale of many acronyms

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USRA project under supervision of Carl Michal and Alex MacKay

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Goal+Motivation

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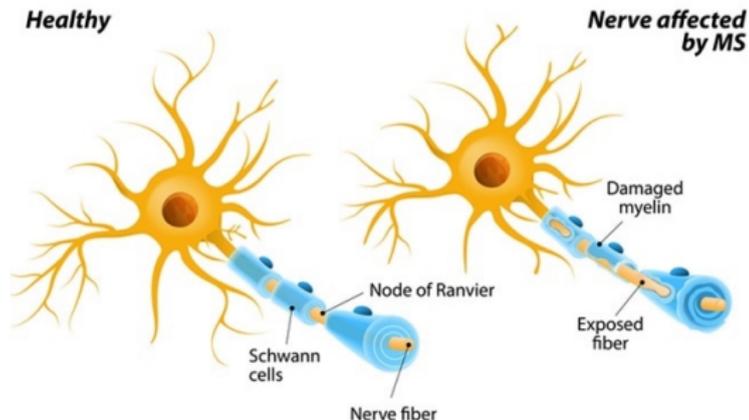


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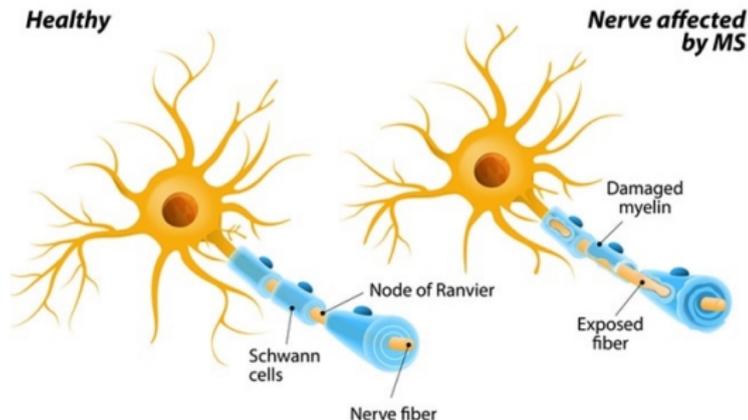


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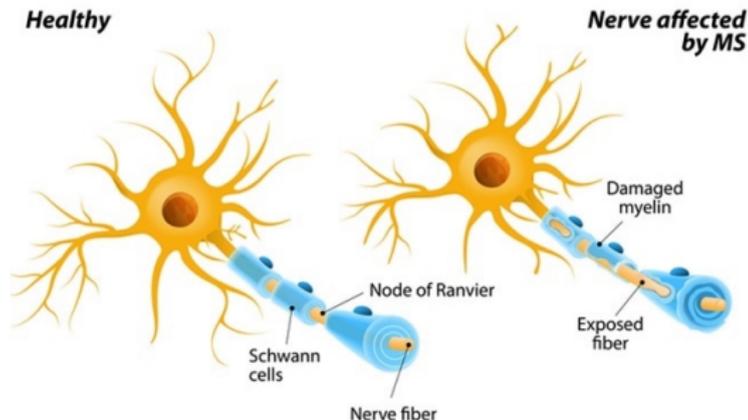


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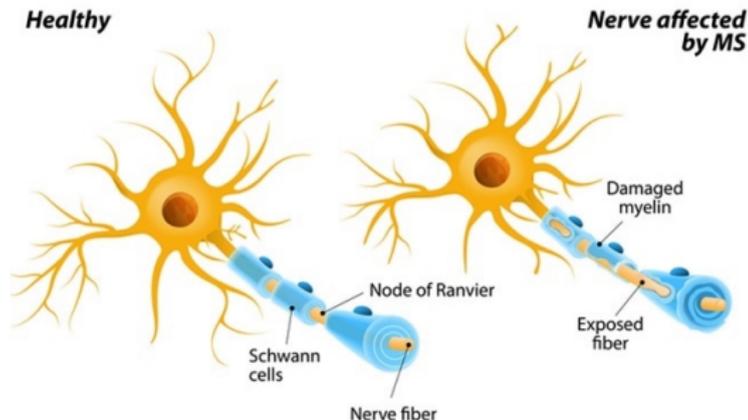


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- ▶ More selective technique: ihMT!
- ▶ In this talk: New method of ihMT with pseudo-random noise sequences.

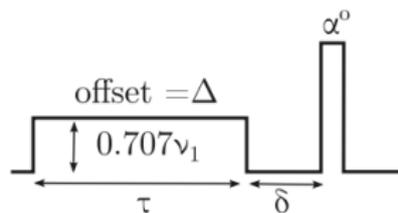
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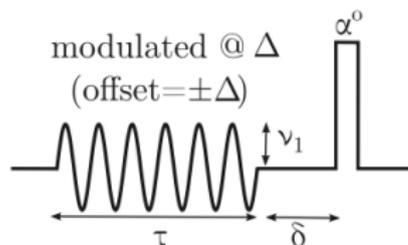
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ihMT: S_+ , S_- , S_0 ($\nu_1=0$)

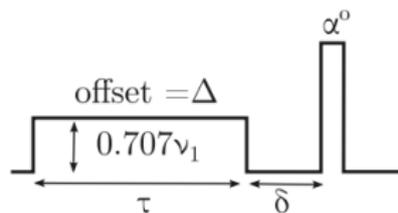


ihMT: S_{dual}

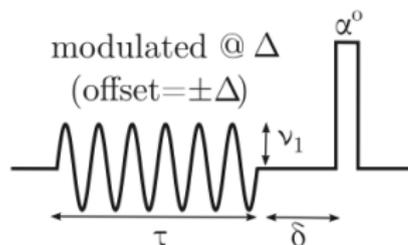
Image taken from A.P. Manning et al., *Journal of Magnetic Resonance*, 274 (2017) 125–136

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ihMT: S_+ , S_- , S_0 ($\nu_1=0$)



ihMT: S_{dual}

Image taken from A.P. Manning et al., *Journal of Magnetic Resonance*, 274 (2017) 125–136

- We can then define the ihMT ratio as:

$$\text{ihMTR} = \frac{S_+ + S_- - 2S_{\text{dual}}}{2S_0}$$

What is ihMT? II

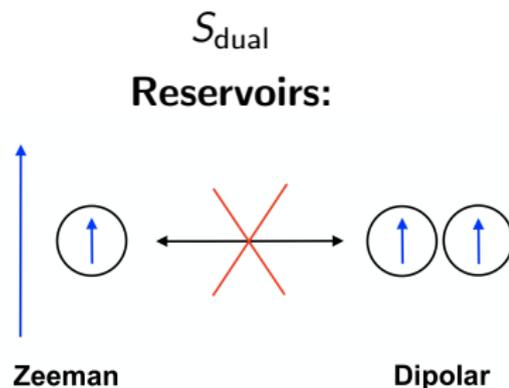
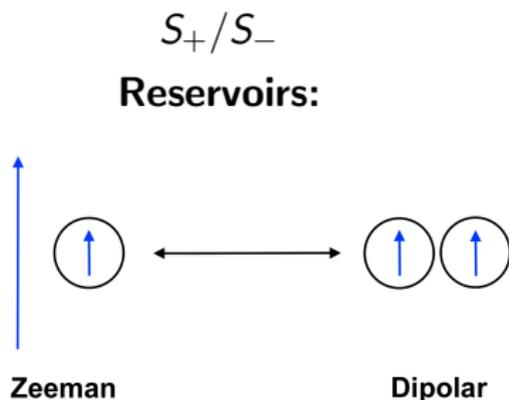
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$$S_+/S_-$$

$$S_{\text{dual}}$$

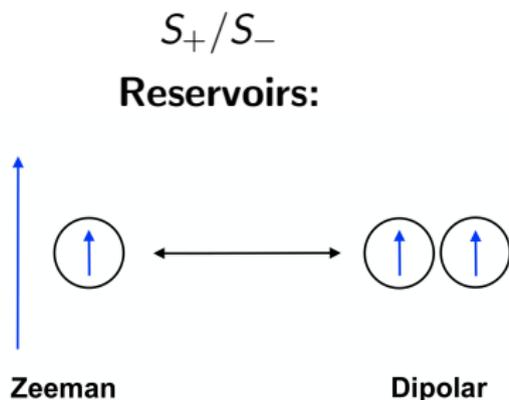
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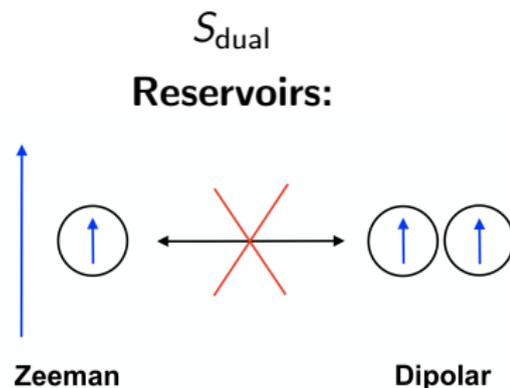


What is ihMT? II

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Spectrum: Asymmetry
from dipolar order.



Spectrum: Symmetric
suppression on both sides.

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- ▶ For long T_{1D} , $S_{+/-} > S_{\text{dual}}$ and ihMT can be measured.
- ▶ Lipid bilayers have long T_{1D} due to slow spin diffusion along lipid tails; so in brain tissue, only myelin/glia cells should have a non-negligible ihMT signal.

Maximum-Length Binary Sequences

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- ▶ $2^k - 1$ length binary sequence

Maximum-Length Binary Sequences

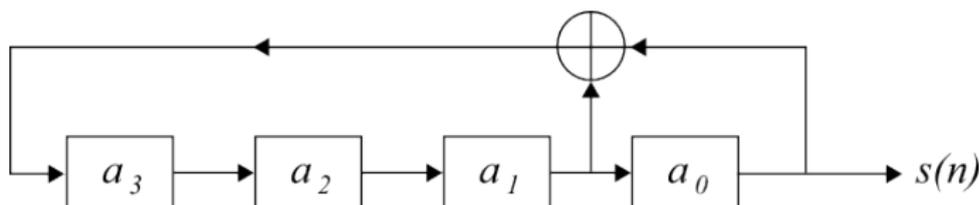
- ▶ $2^k - 1$ length binary sequence
- ▶ For k shift registers, we can produce the MLBS via:

$$\left\{ \begin{array}{l} s[n] = a_0[n] \\ a_k[n+1] = a_0[n] + a_1[n] \pmod{2} \\ a_{k-1}[n+1] = a_k[n] \\ \vdots \\ a_1[n+1] = a_2[n] \\ a_0[n+1] = a_1[n] \end{array} \right.$$

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- ▶ Flat power spectrum, distributed over $\frac{1}{T_{MLBS}}$
- ▶ **Idea:** MLBS' can be used for in low (power) cost pulse sequences for observing ihMT.

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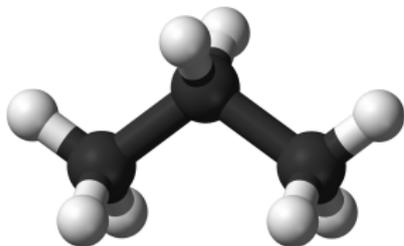


- ▶ Backup plan: simulations with SIMPSON (SIMulation Program for SOLid-state NMR)!

Setup + Early tests

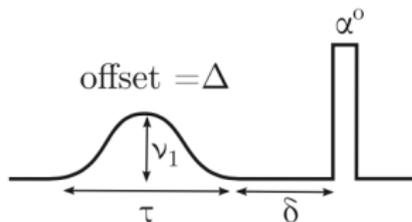
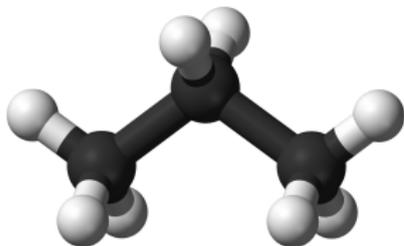
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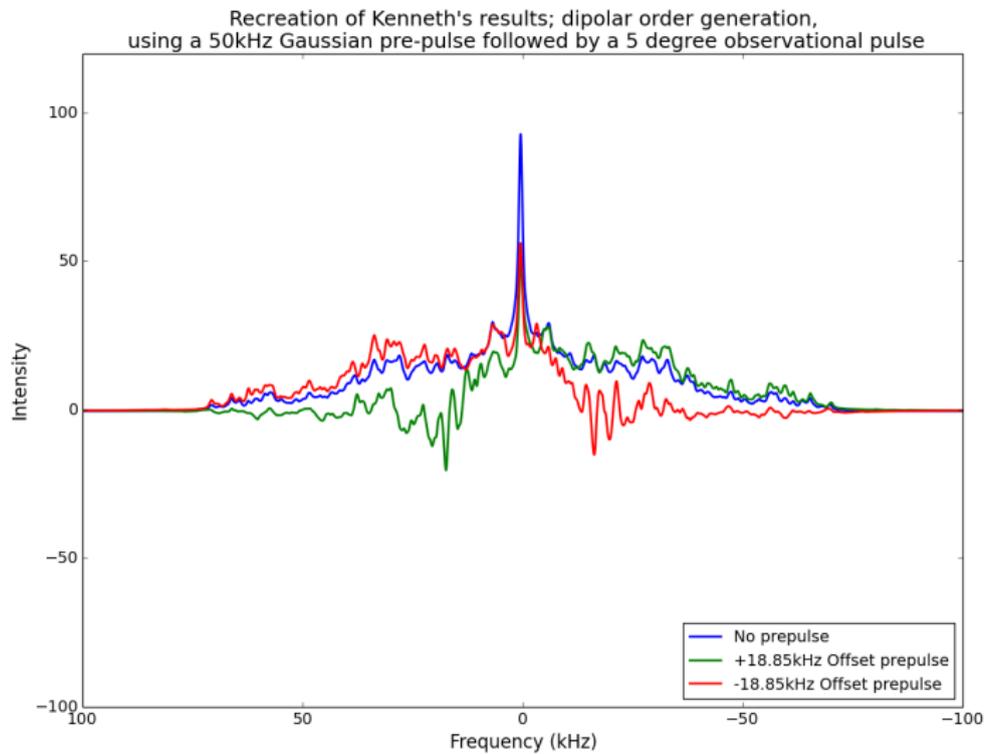
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Dipolar order
creation

Image taken from A.P. Manning et al., *Journal of Magnetic Resonance*, 274 (2017) 125–136

Setup + Early tests II



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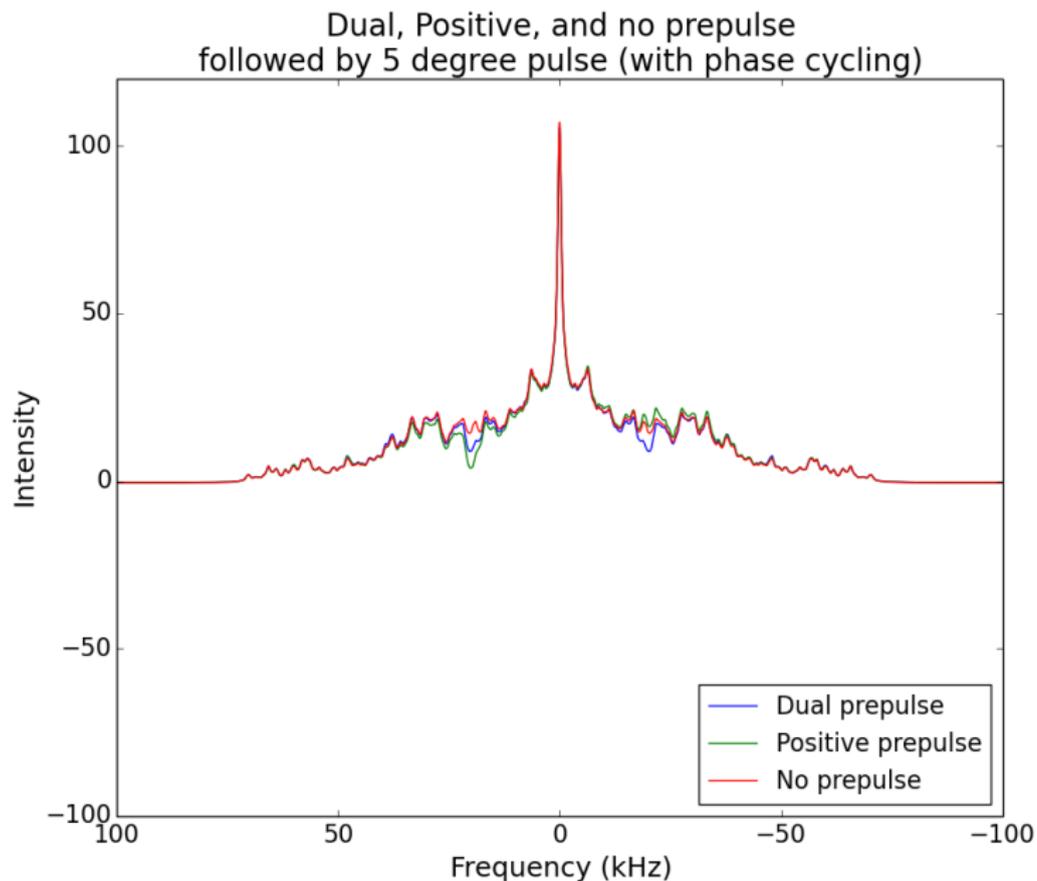
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Exp.#	Prep. phase	Obs. pulse phase	Receiver phase
1	-x	-x	y
2	-x	-y	-x
3	-x	x	-y
4	-x	y	x

Setup + Early Tests IV



From the continuous to the pseudo-random

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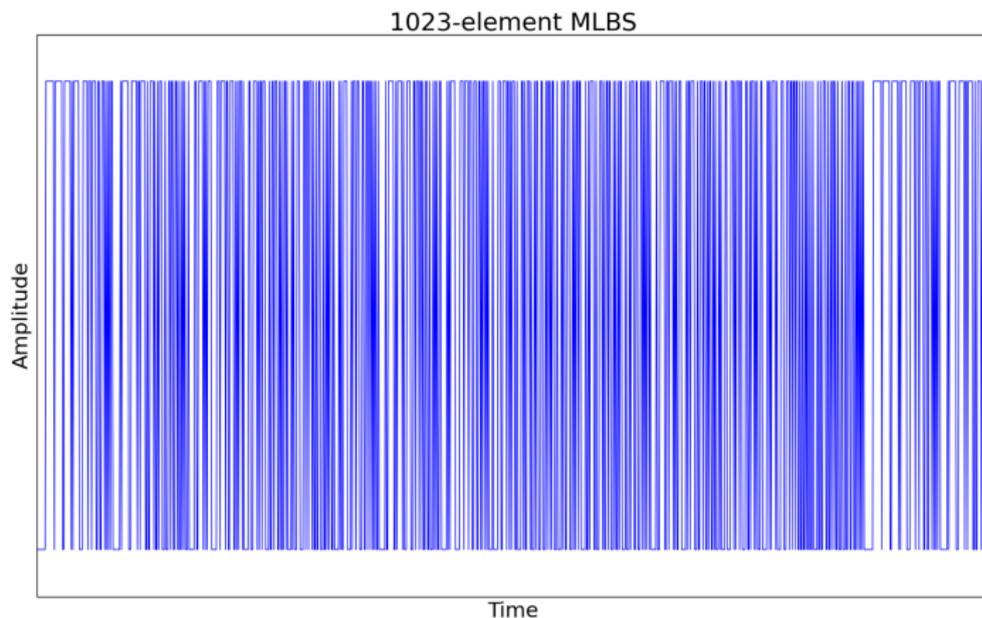
- ▶ Dual prepulse \rightarrow MLBS prepulse

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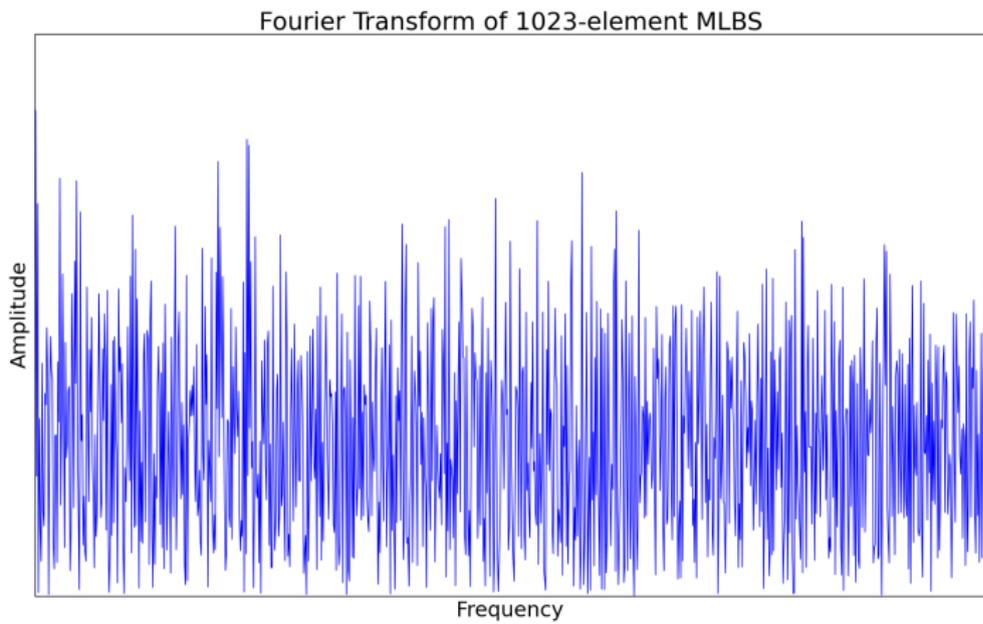
- ▶ Dual prepulse \rightarrow MLBS prepulse
- ▶ How do we create S_+/S_- with MLBS' ?

Physicists hate him!

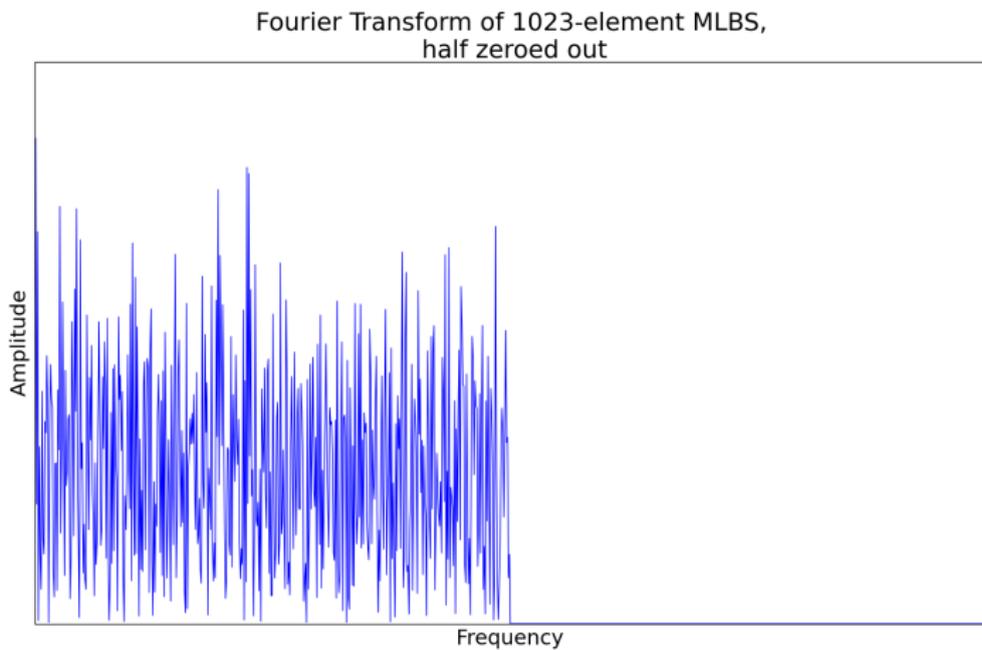
Three simple steps to create dipolar order with your MLBS



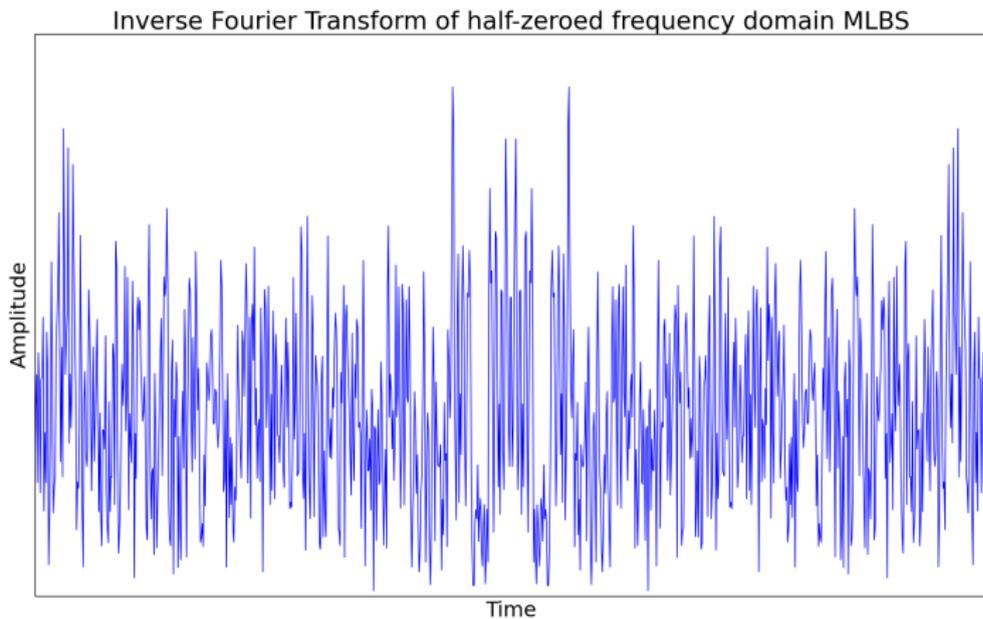
Step 1



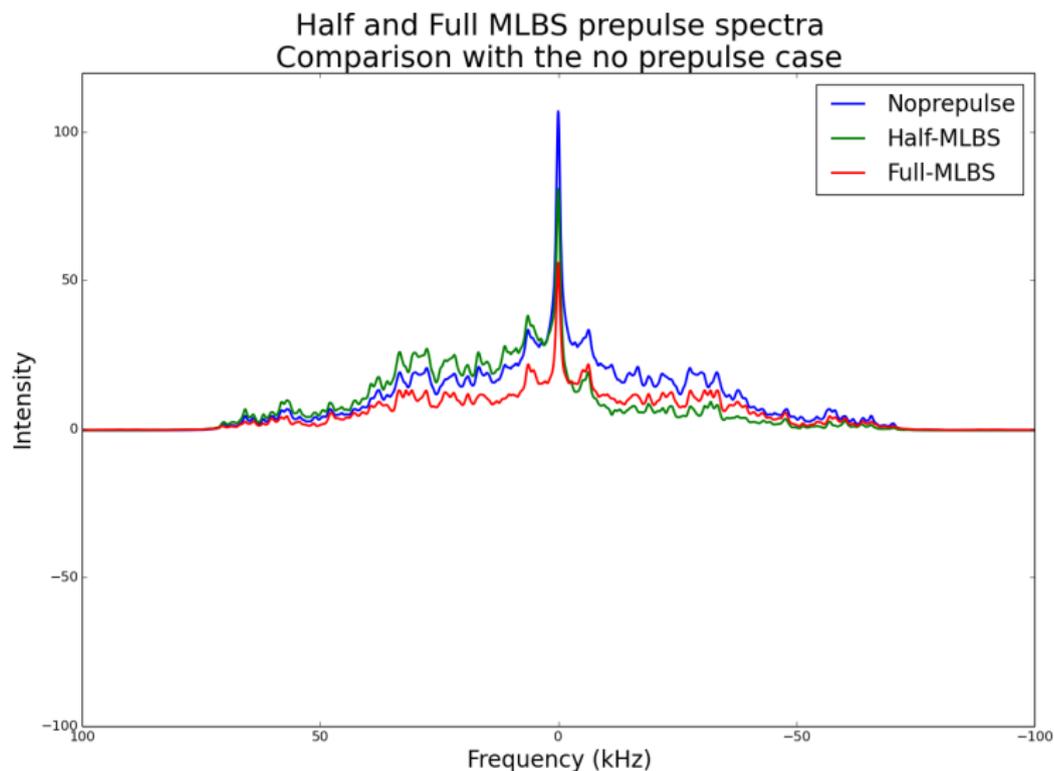
Step II



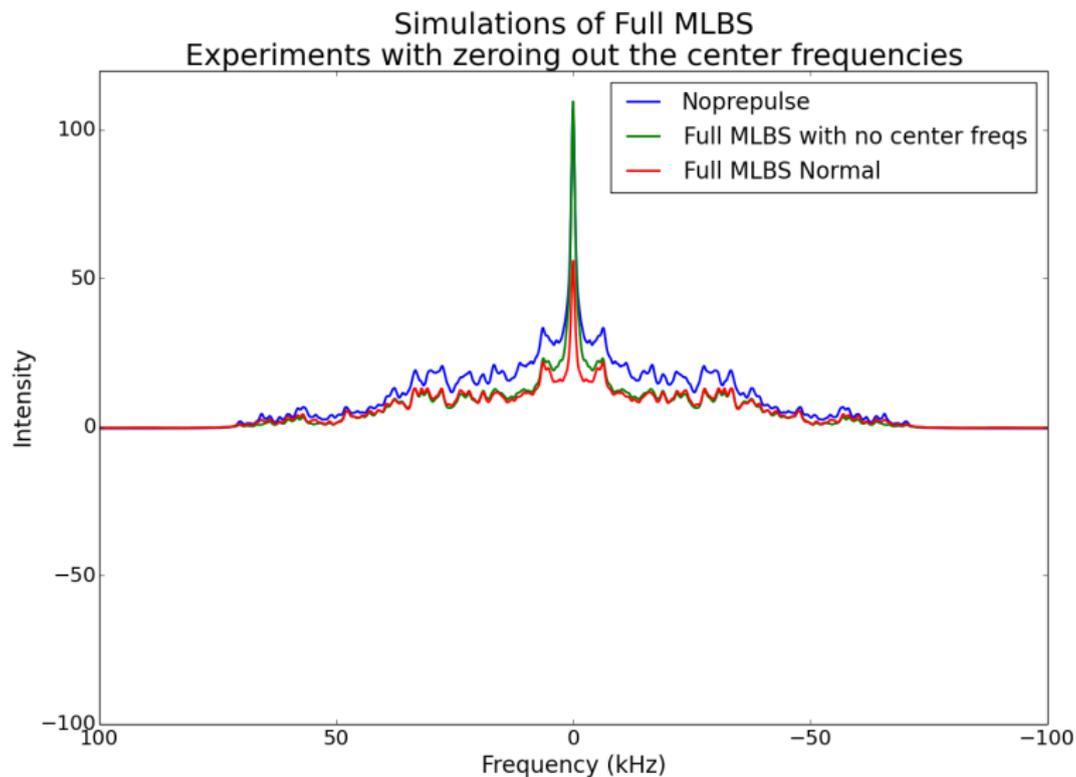
Step III



Full/Half-MLBS spectra



Selective removal of (center) frequency points



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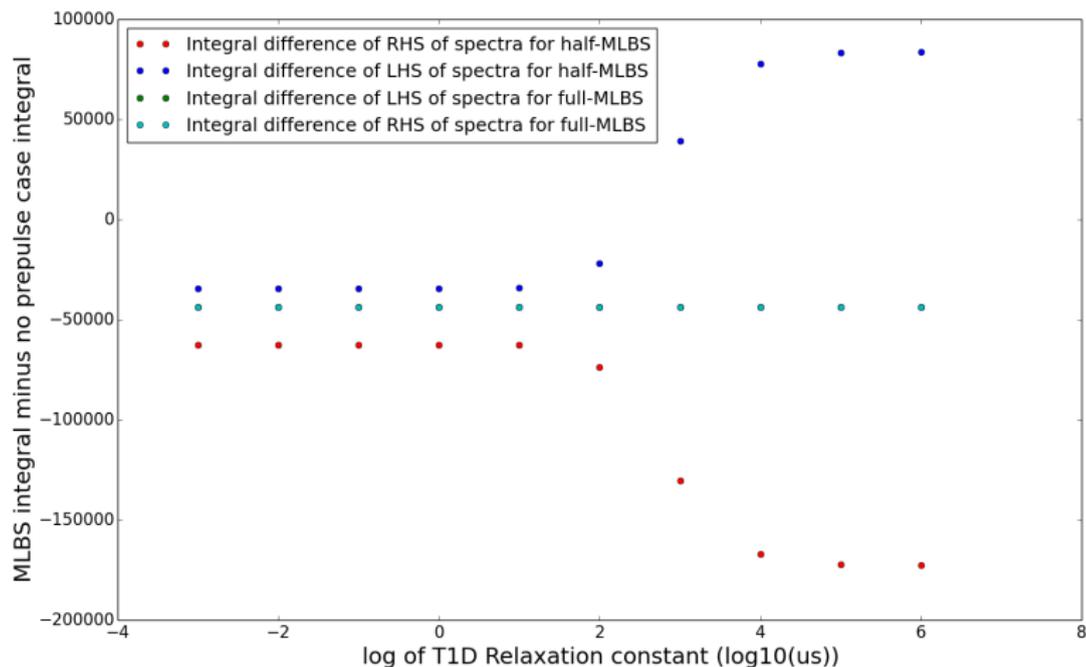
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- ▶ This part of the density matrix can be relaxed:

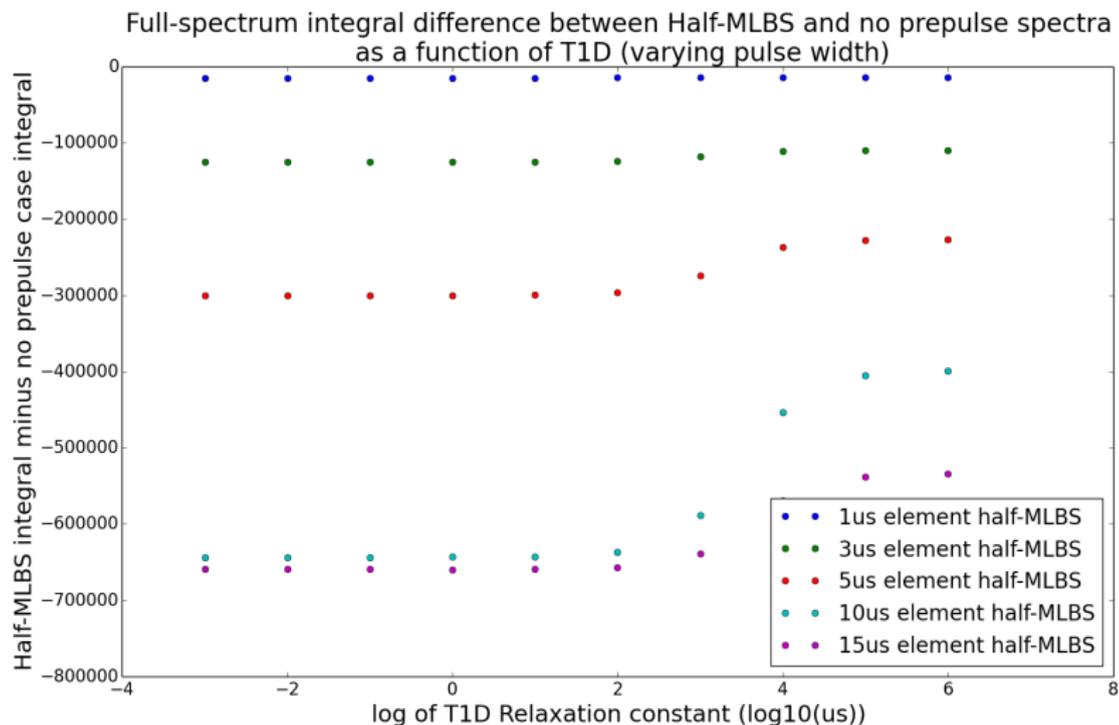
$$\rho_{\text{dipole}} * \exp\left(-\frac{\Delta t}{\tau}\right)$$

T1D dependence of spectra

Integral difference (between MLBS and no prepulse spectra) vs. log of T1D relaxation time



Varying the MLBS pulsewidth



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- ▶ Removing individual coherence orders from the spectrum → Learned that spectrum depends solely on order 0.

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- ▶ 1. At each time step, remove all of the I_z parts of the density matrix; i.e. for each spin i :

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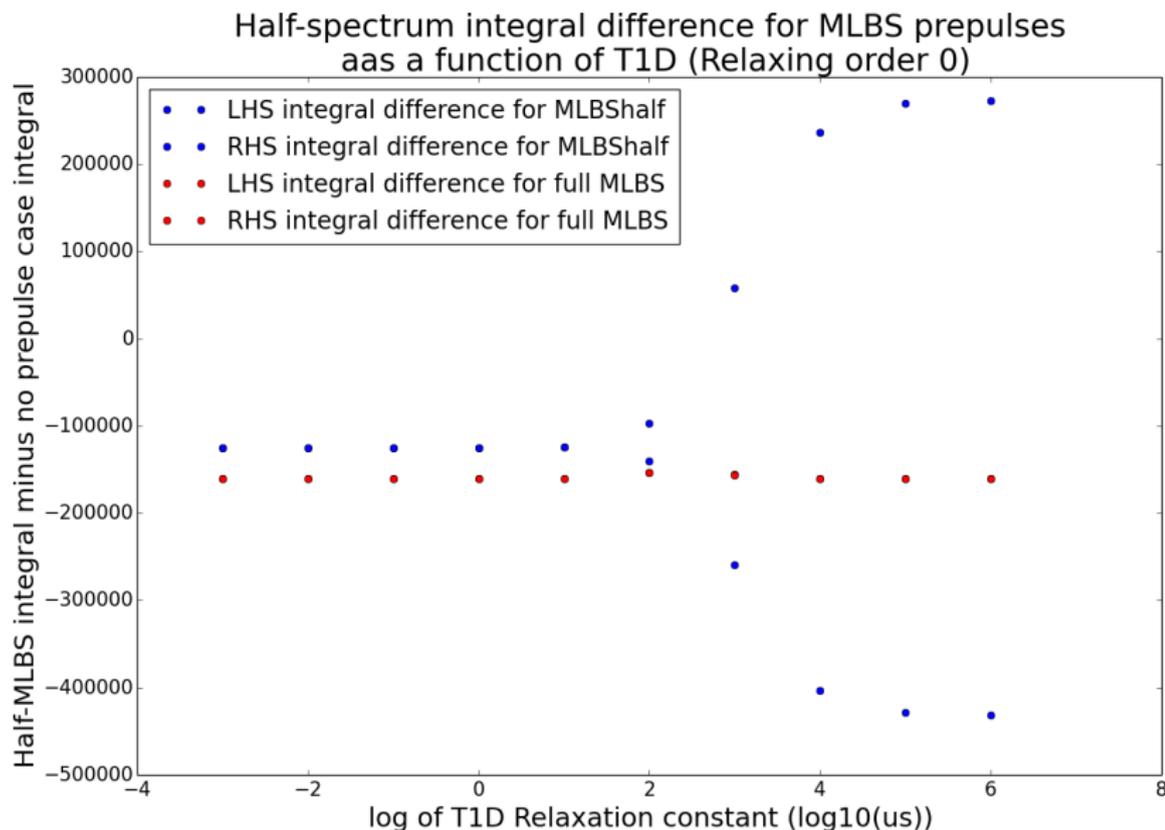
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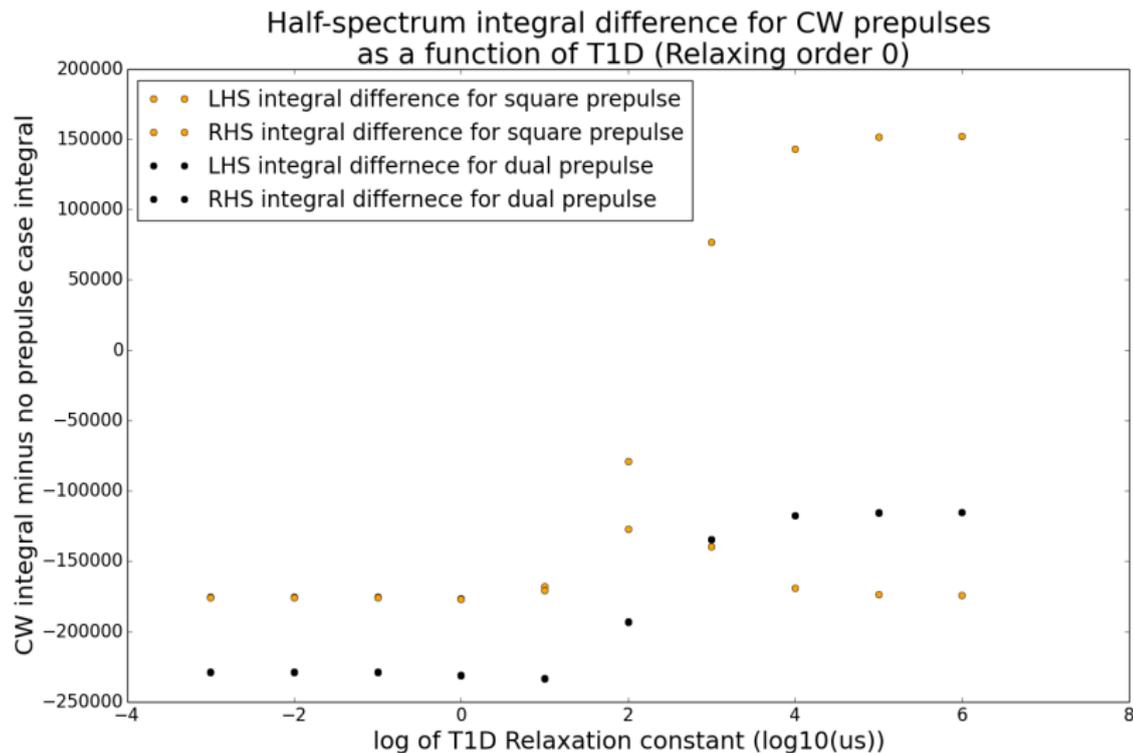
$$\rho_{\text{Order } 0} * \exp\left(-\frac{\Delta t}{\tau}\right)$$

- ▶ 3. Add back in the I_z parts, and continue the pulse sequence.

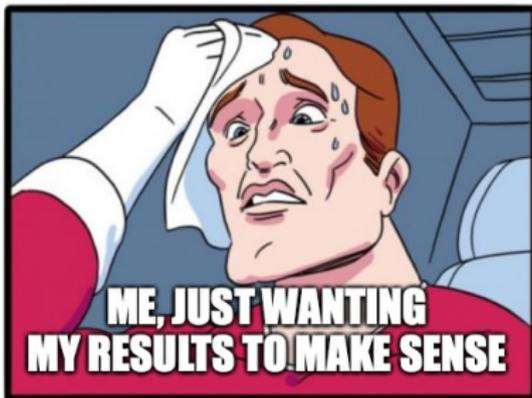
Spectra from new relaxation method - MLBS



Spectra from new relaxation method - CW



How do we make the system relax?



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- ▶ Developing a comparison between the MLBS prepulse and the CW prepulse cases; which is more efficient?
- ▶ Possible new directions: Coloured Frank sequences, hyperbolic secant pulses?
- ▶ Running experiments remotely?

It's alright to be uncertain...

```
/** would this work??? */  
for (i=0; i<NN; i++) {  
    is = i % sim->Nfstart;  
    id = i % sim->Nfdetect;  
    // basis compatibility check  
    if (wsp->fdetect[id]->basis != wsp->sigma[is]->basis) {  
        mat_complex *dum = cm_change_basis_2(wsp->fdetect[id],wsp->sigma[is]->basis,sim  
        if (wsp->fdetect[id] != sim->fdetect[id]) free_complex_matrix(wsp->fdetect[id]  
        wsp->fdetect[id] = dum;  
    }  
    if (sim->acq_adjoint == 0) {  
        z = cm_trace(wsp->fdetect[id],wsp->sigma[is]);  
    } else {  
        z = cm_trace_adjoint(wsp->fdetect[id],wsp->sigma[is]);  
    }  
    ptr = &(wsp->fid[wsp->curr_nsig+i*sim->ntot]);  
    if (fabs(phase) > TINY) {  
        ptr->re += phfac.re*z.re+phfac.im*z.im;  
        ptr->im += -phfac.im*z.re+phfac.re*z.im;  
    } else {  
        ptr->re += z.re;  
        ptr->im += z.im;  
    }  
}
```