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MASTER THESIS: BUILDING A 25 MHZ NMR SPECTROMETER

Maximilian Stabel

September 12, 2023

ETH Zürich

2023-09-12

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“What I cannot create, I do not understand”

—Richard Feynman

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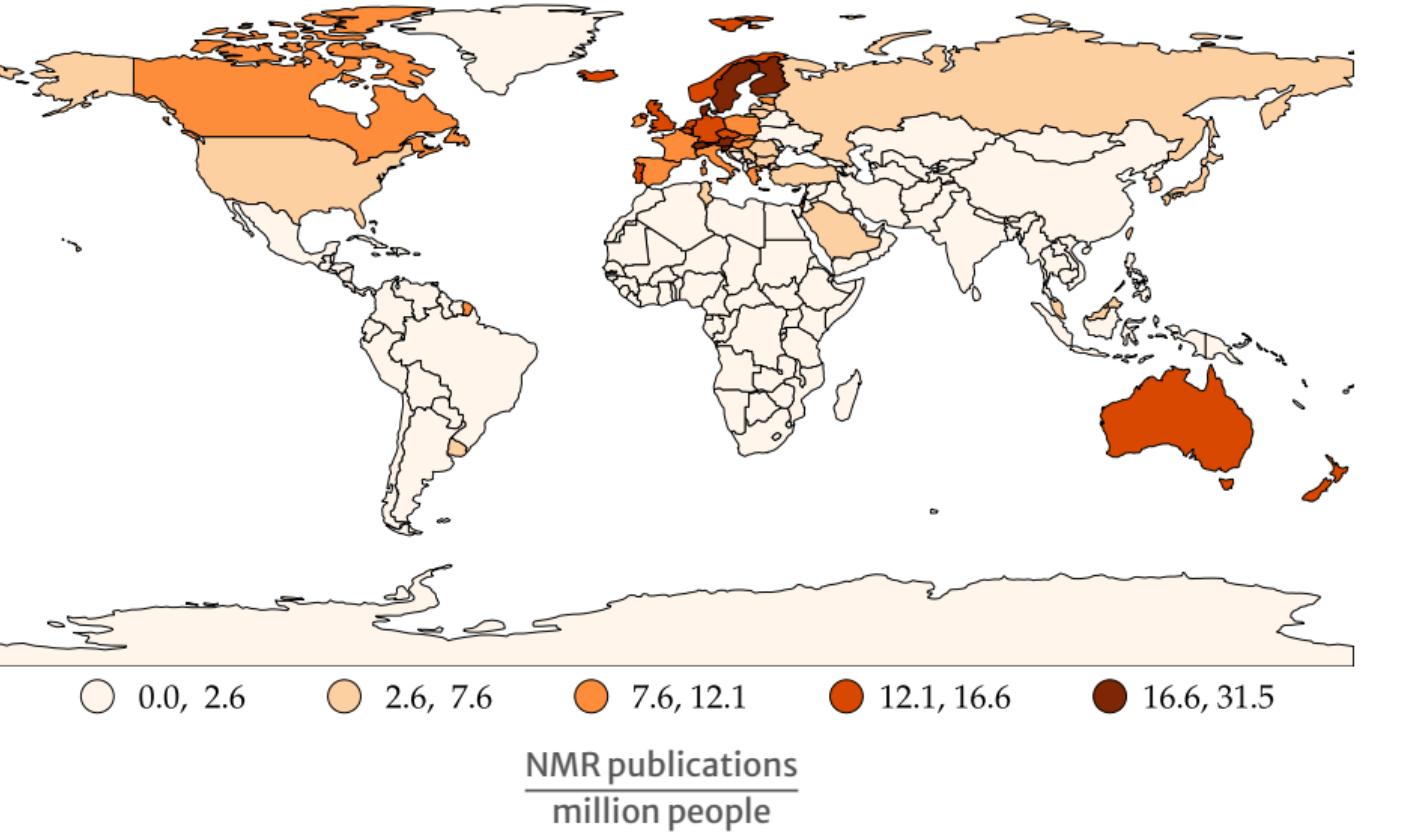
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“What I cannot create, I do not understand”

—Richard Feynman

1. In the spirit of Richard Feynman...
2. My master thesis is about building an NMR spectrometer
3. I'm Max and I'll be your host for today
4. Speaking of understanding...

There is not a lot of NMR research in the Global South



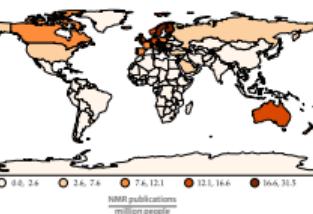
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There is not a lot of NMR research in the Global South

Reminder: What is NMR spectrometer

There is not a lot of NMR research in the Global South



Nuclear Magnetic Resonance

- Nuclei absorb radio waves at a certain frequency when inside a magnetic field
- The nuclei emit radio waves at that same frequency when excited this way
- $f \sim B_0$ and surroundings

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└ Nuclear Magnetic Resonance

- You: Understanding for own experiments
- The better we know the better we can use
- Push NMR development — better machines
- Transition: if not about you personally — more globally: applications

- Nuclei absorb radio waves at a certain frequency when inside a magnetic field
- The nuclei emit radio waves at that same frequency when excited this way
- $f \sim B_0$ and surroundings

NMR is used across various fields

- Research (Structure Analysis, Drug Discovery, ...)
- Medicine (Imaging, Diagnosis, ...)
- Industry (Process Control, Drug screening, ...)
- Education (Quantum Mechanics, Quantum Computing, ...)

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└ NMR is used across various fields

1. Some of you already know, but here are some reasons why NMR is useful

- Research (Structure Analysis, Drug Discovery, ...)
- Medicine (Imaging, Diagnosis, ...)
- Industry (Process Control, Drug screening, ...)
- Education (Quantum Mechanics, Quantum Computing, ...)

**Build an accessible
NMR spectrometer**

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Build an accessible
NMR spectrometer

1. The goal of my thesis was...

Preview

The parts

The complete setup

Experimental Results

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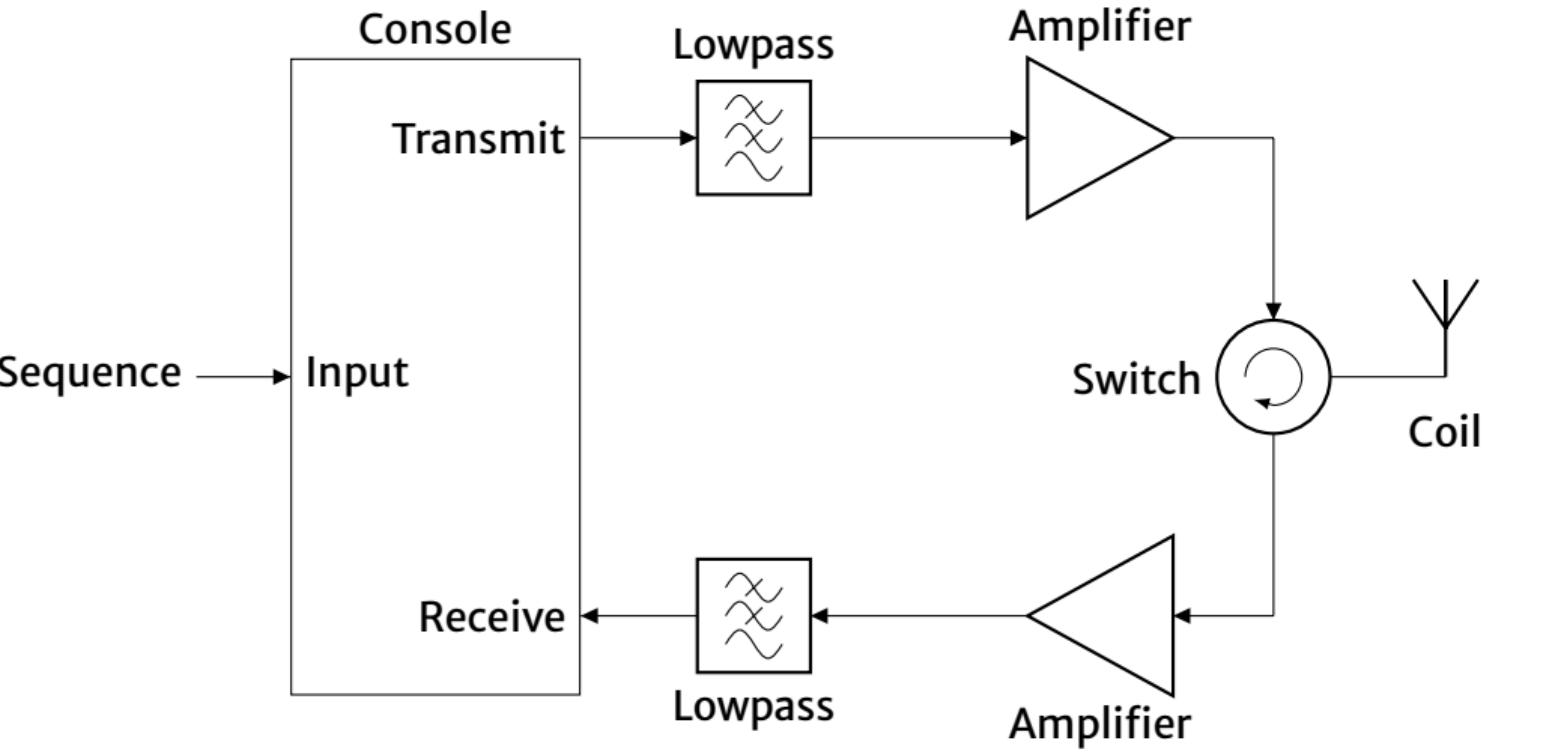
└ Preview

THE PARTS

THE PARTS

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└ The parts

Our goal is to build an accessible NMR spectrometer



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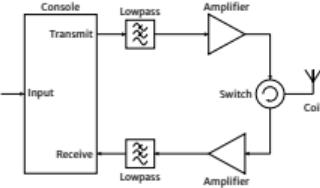
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The parts

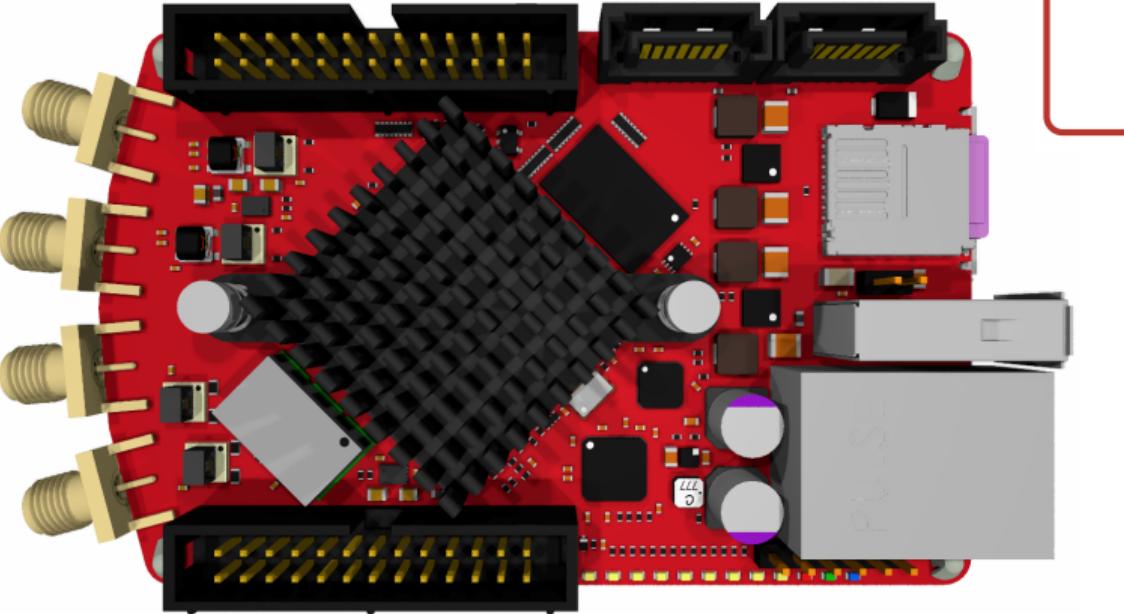
Console
Transmit
Input
Receive
Lowpass
Amplifier
Switch
Coil

1. Go through the parts left to right
2. Our switch only, others might include more analog processing

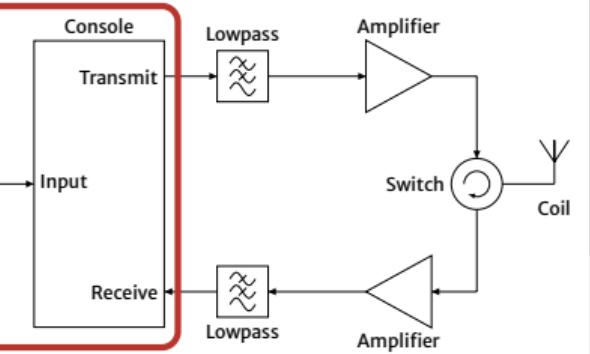
Our goal is to build an accessible NMR spectrometer



The console
is a ready-made FPGA board*



*Red Pitaya SDRlab 122-16



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The parts

1. FPGAs

2. RF Frontend

3. SDR

4. Antennas

5. Power

6. Case

7. Software

8. Tools

9. Magnets

10. Sensors

11. Calibration

12. Processing

13. Results

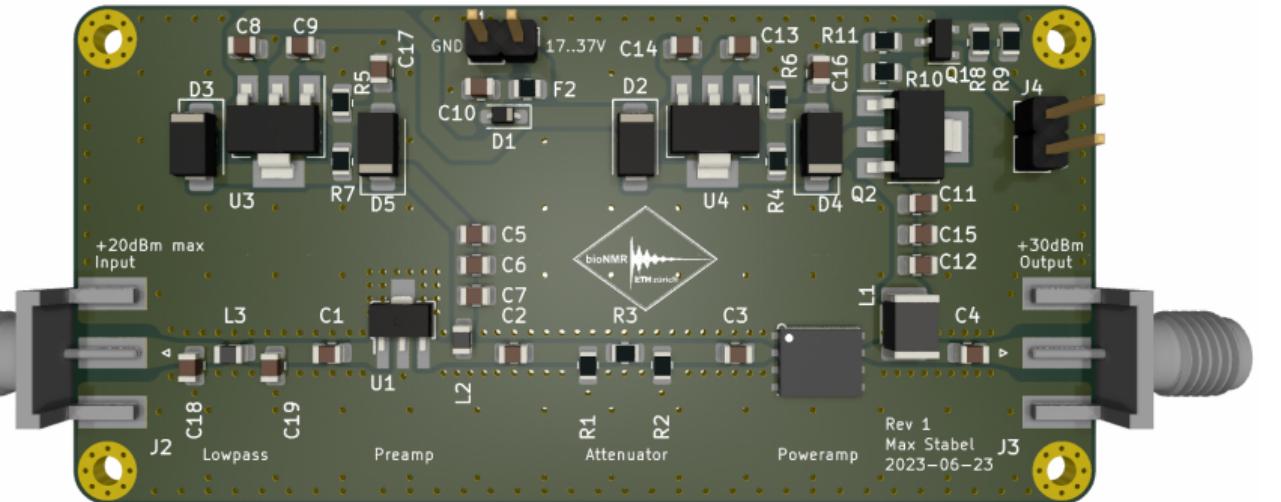
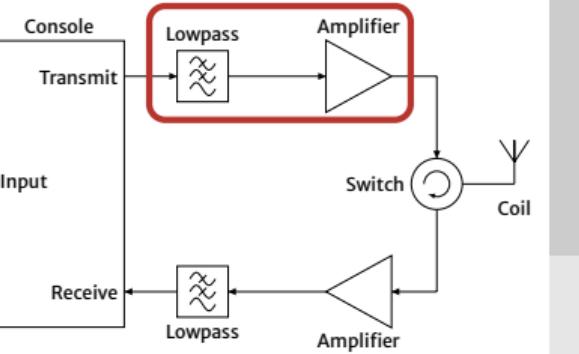
14. Conclusion

15. Questions



The console
is a ready-made FPGA board*

The power amplifier has two stages



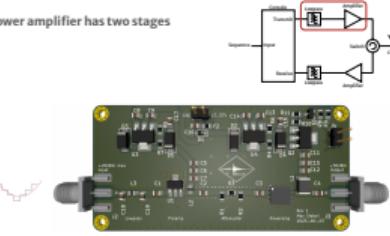
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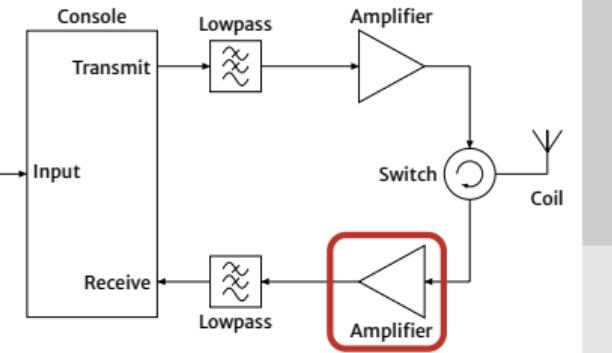
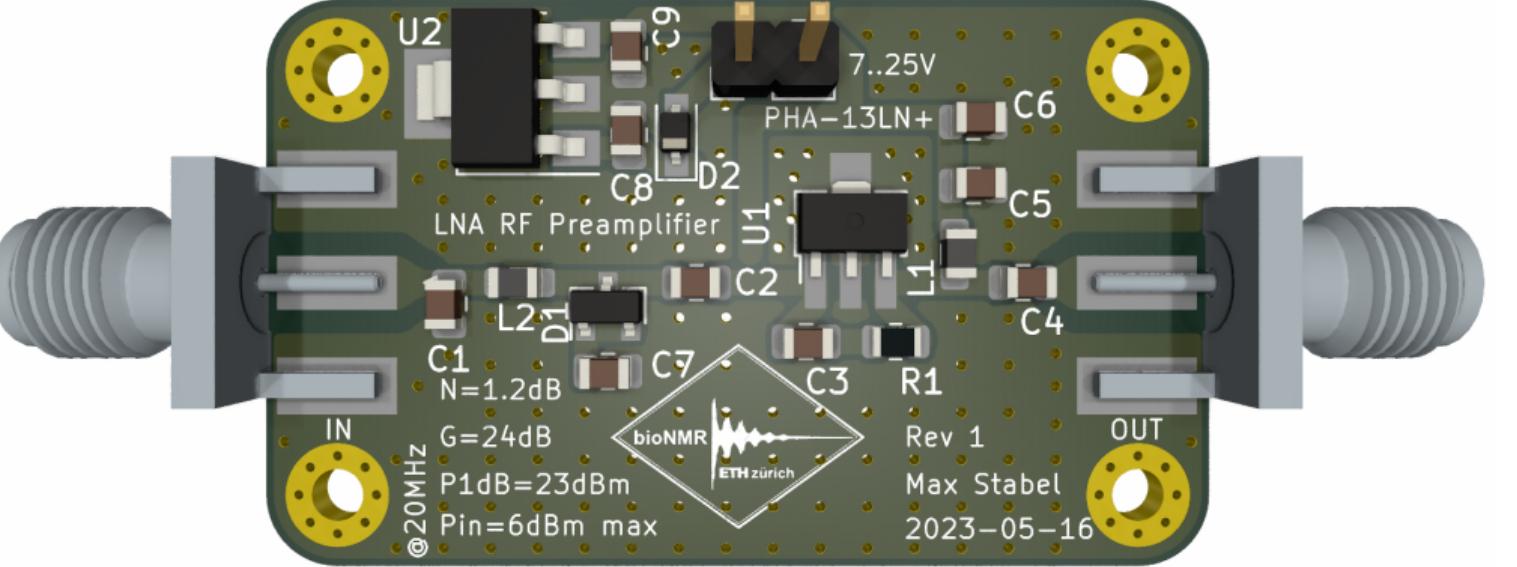
The parts

Power amplifier

1. We want cheap, so using a simple is the obvious first approach
2. Unfortunately there's a lot to do:
 - Input/Output Impedance Matching
 - Bias Tee
 - DC coupling
 - stability calculations
 - feedback
 - temperature compensation (current feedback)
3. A complete amplifier is quite expensive
4. Solution: Use monolithic (integrated) amplifier
5. Take care of heat dissipation (Class-A)
6. dB is logarithmic unit



The low-noise amplifier had instability issues

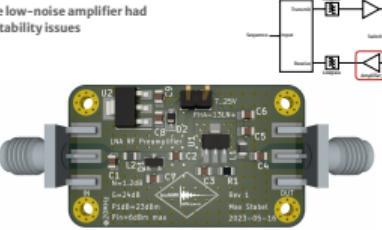


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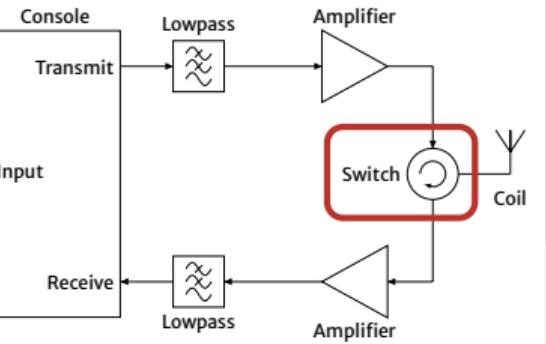
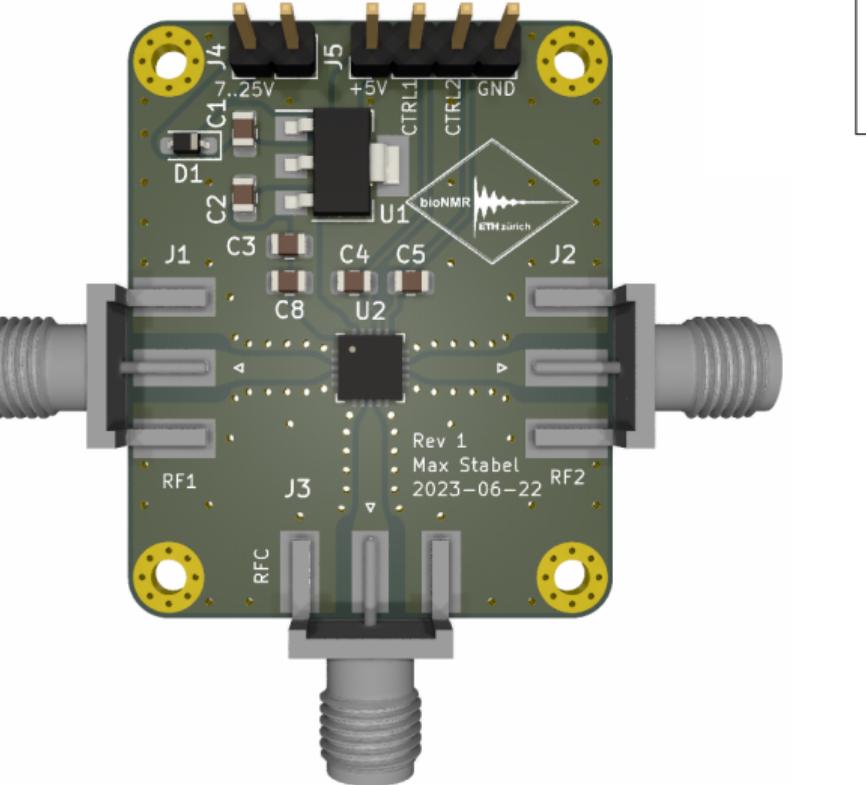
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The parts

1. Low-noise
2. Feedback loop — stray capacitance
3. Solution: Smaller housing, shorter loop
4. We need 3x for enough gain



We use a transistor-based active switch

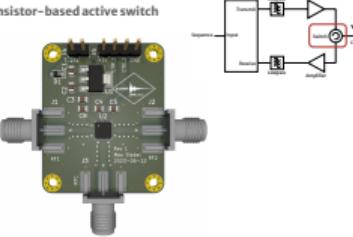


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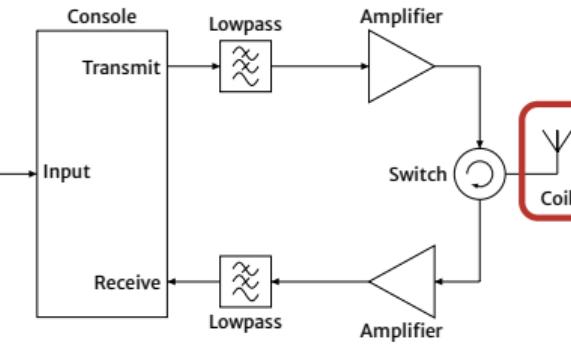
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The parts

1. Active
2. Isolation: 60 dB
3. Silicon-on-insulator (not pHEMT GaAs) i.e. FET tech, not PIN-Diode
4. PIN-Diode switch also possible, but
 - usually higher leakage
 - slower switching
 - harder to integrate on a chip
 - but higher power capabilities



The probe

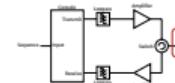


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The parts

1. Many turns — high inductance — low capacitance — sensitive to stray capacitance



A 32-channel current supply is designed but untested



m
□

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The parts

The parts

100 | Page

current supply is designed but untested



THE COMPLETE SETUP

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└ The complete setup

THE COMPLETE SETUP

Our NMR is affordable ...

	600 MHz†	mini-circuits	<i>magnETHical</i>
Power Amplifier	50 000	323.49	36.01
Switch	-	82.06	20.05
Probe	100 000	-	≈15.00
Low-Noise Amplifier	50 000	409.38	73.11
Shim Driver	-	-	257.08
Console	200 000	-	662.53
Magnet	1 000 000	-	≈9000.00
Sum			10 142.80

[†]estimated costs

Prices incl. VAT [CHF]

n
□

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—The complete setup

| C-NMR: ff-III

	600 MHz ^f	mini-circuits	magnETHICal
Power Amplifier	50 000	323.49	36.01
Switch	-	82.06	20.05
Probe	100 000	-	=15.00
Low-Noise Amplifier	50 000	409.38	73.11
Shim Driver	-	-	257.08
Console	200 000	-	662.53
Magnet	1 000 000	-	=9000.00
Sum			10 142.80
estimated costs			
(standard VAT 17%)			

... competitive ...

	Superconducting	Benchtop	<i>magnETHical</i>
Price [k CHF]	200–18 000	50–150	≈10
Frequency [MHz]	300–1200	40–125	25
Resolution [Hz]	≈0.2	0.2–1	≈2.5/50 [†]
Weight [kg]	600–15 000	25–150	≈5

[†]with/without shims

For 5mm standard NMR tubes

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The complete setup

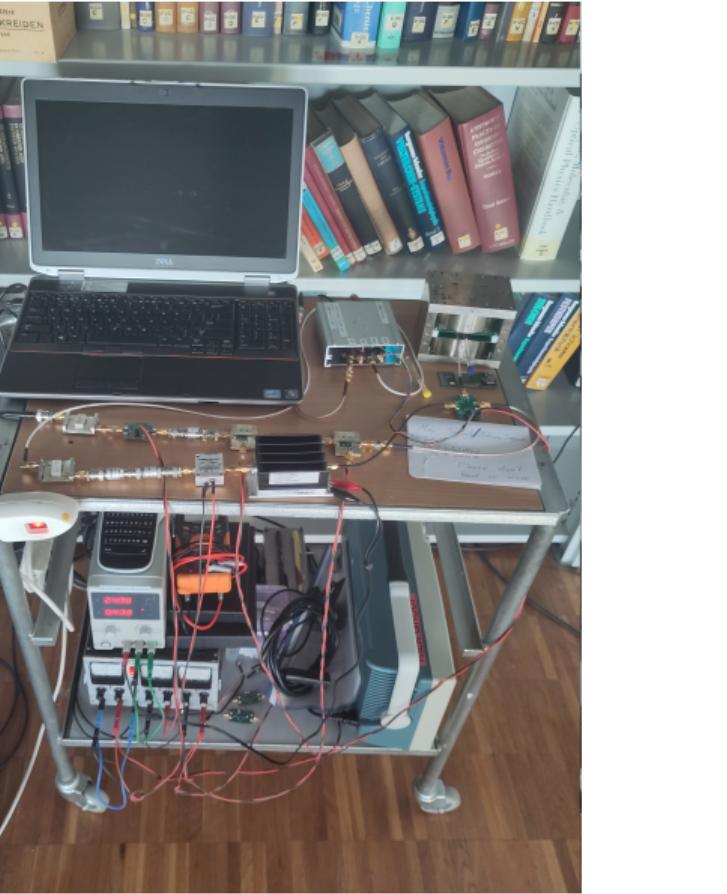
| ...

... competitive ...

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With/without shims
For 5mm standard NMR tubes

... and portable



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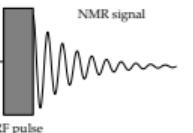
└ The complete setup



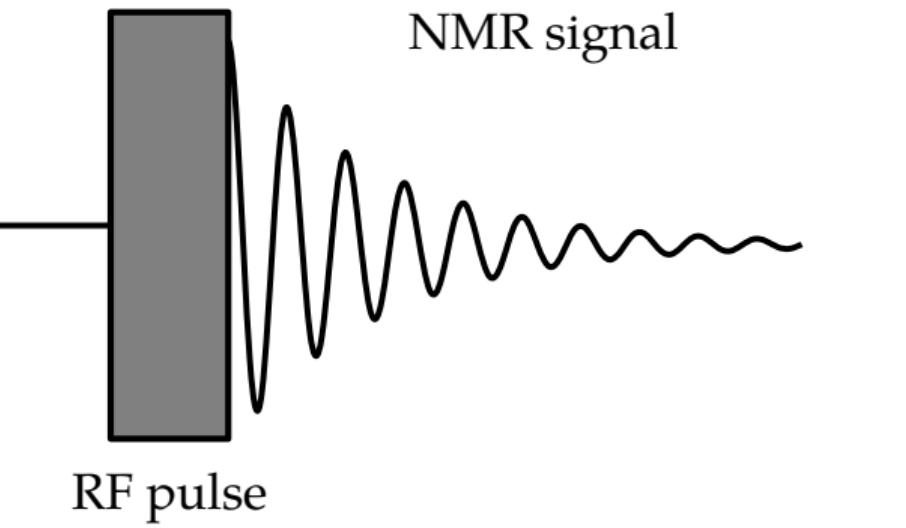
EXPERIMENTAL RESULTS

EXPERIMENTAL RESULTS

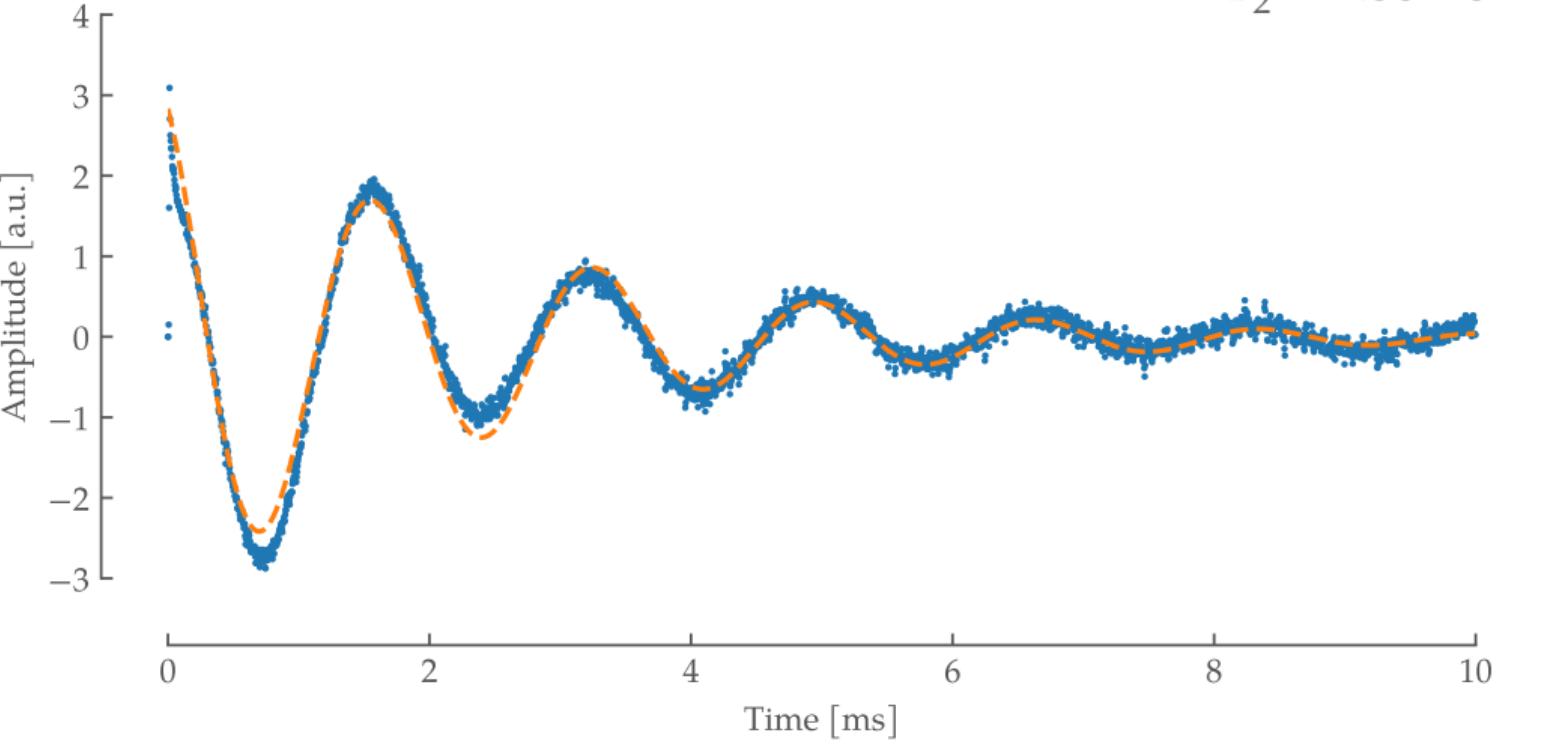
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└ Experimental Results



Simple Pulse Sequence



We can already see a water FID

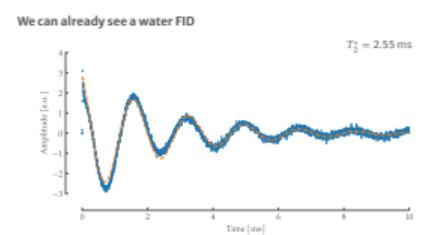


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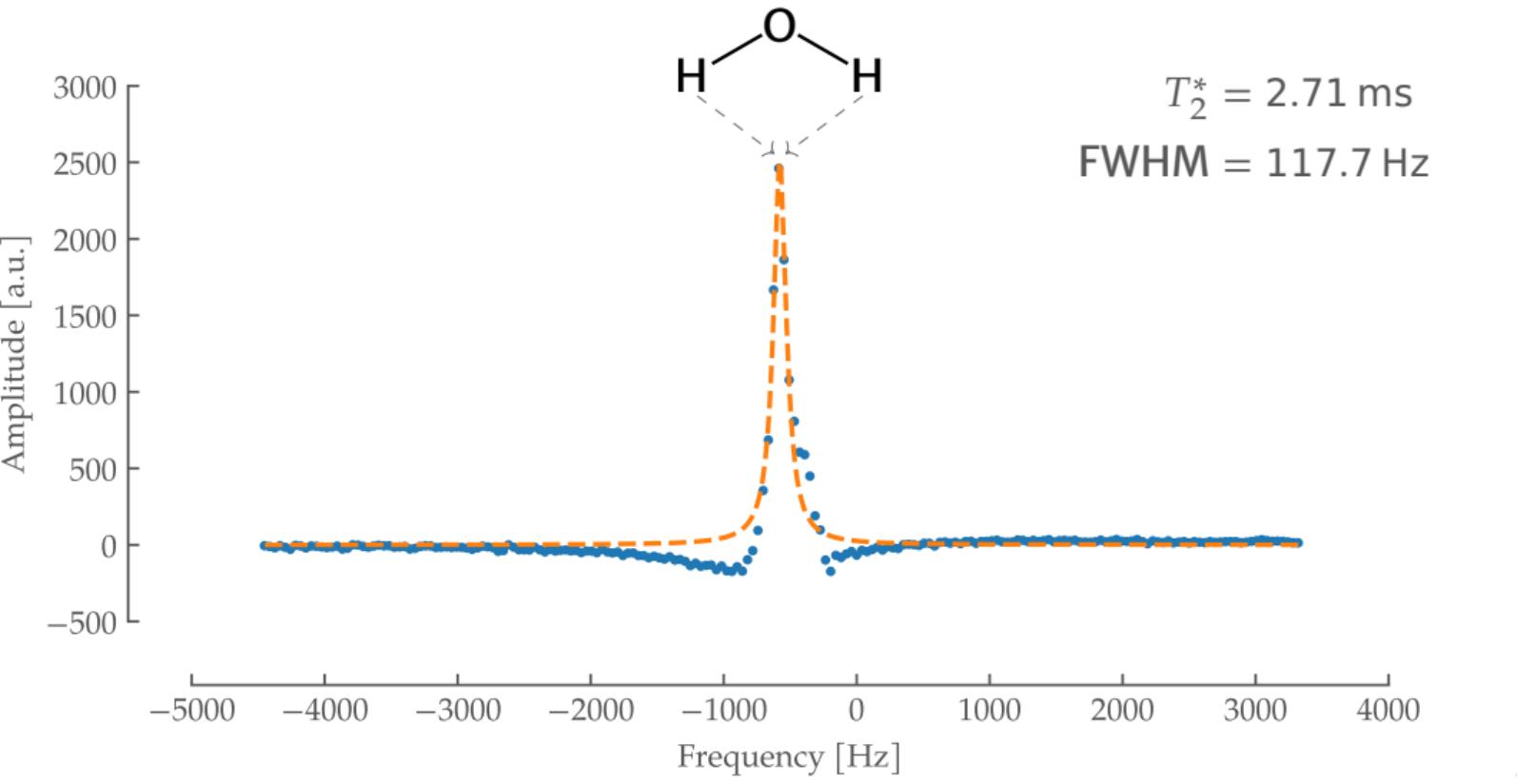
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└ Experimental Results

1. Outliers at the beginning are due to CIC filters



...and do a Fourier transform

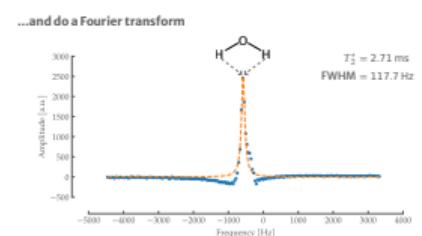


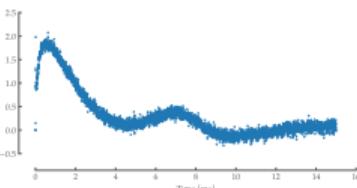
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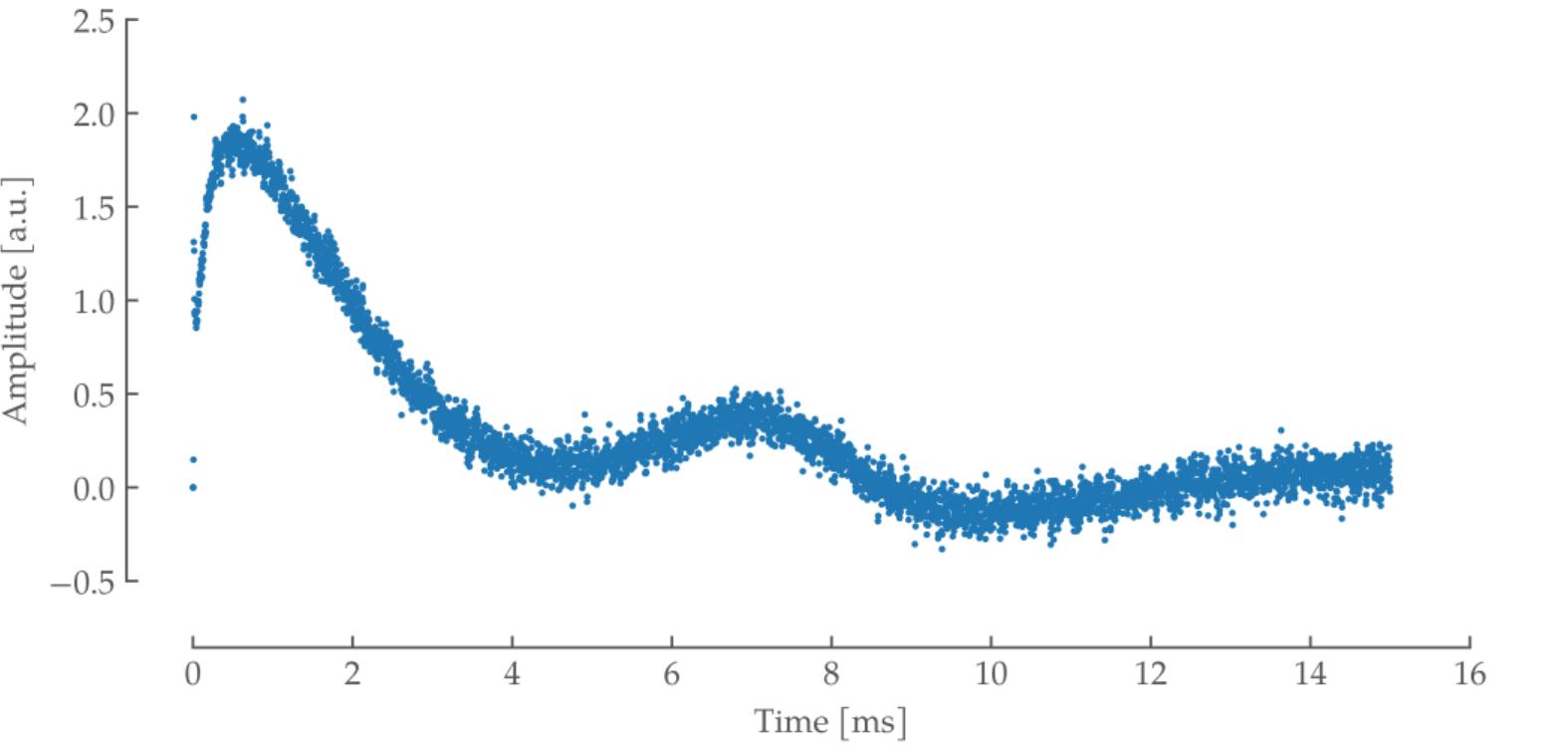
└ Experimental Results

1. Not Lorentz because of missing shimming/inhomogeneities
2. Measured input signal of -92dBm/15.8uV resulted in amplitude of 2200
3. SNR of around 350, With FWHM 2.5Hz/1ppm we estimate snr of 11000





Toluene also has a visible signal

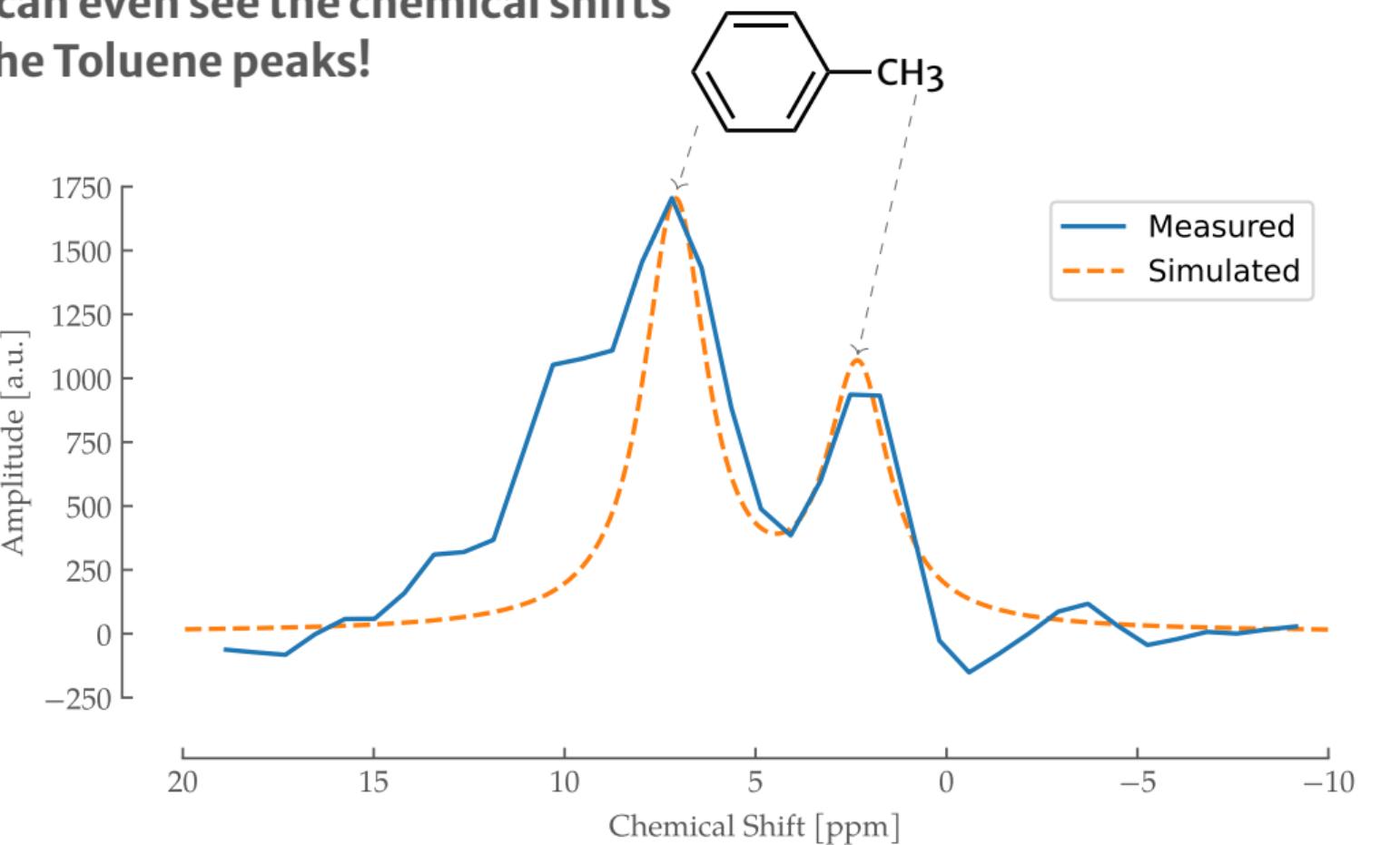


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└ Experimental Results

We can even see the chemical shifts
of the Toluene peaks!



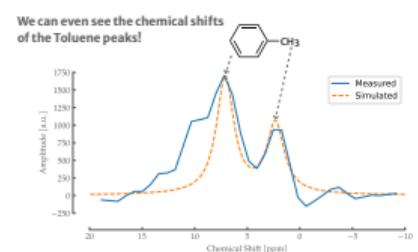
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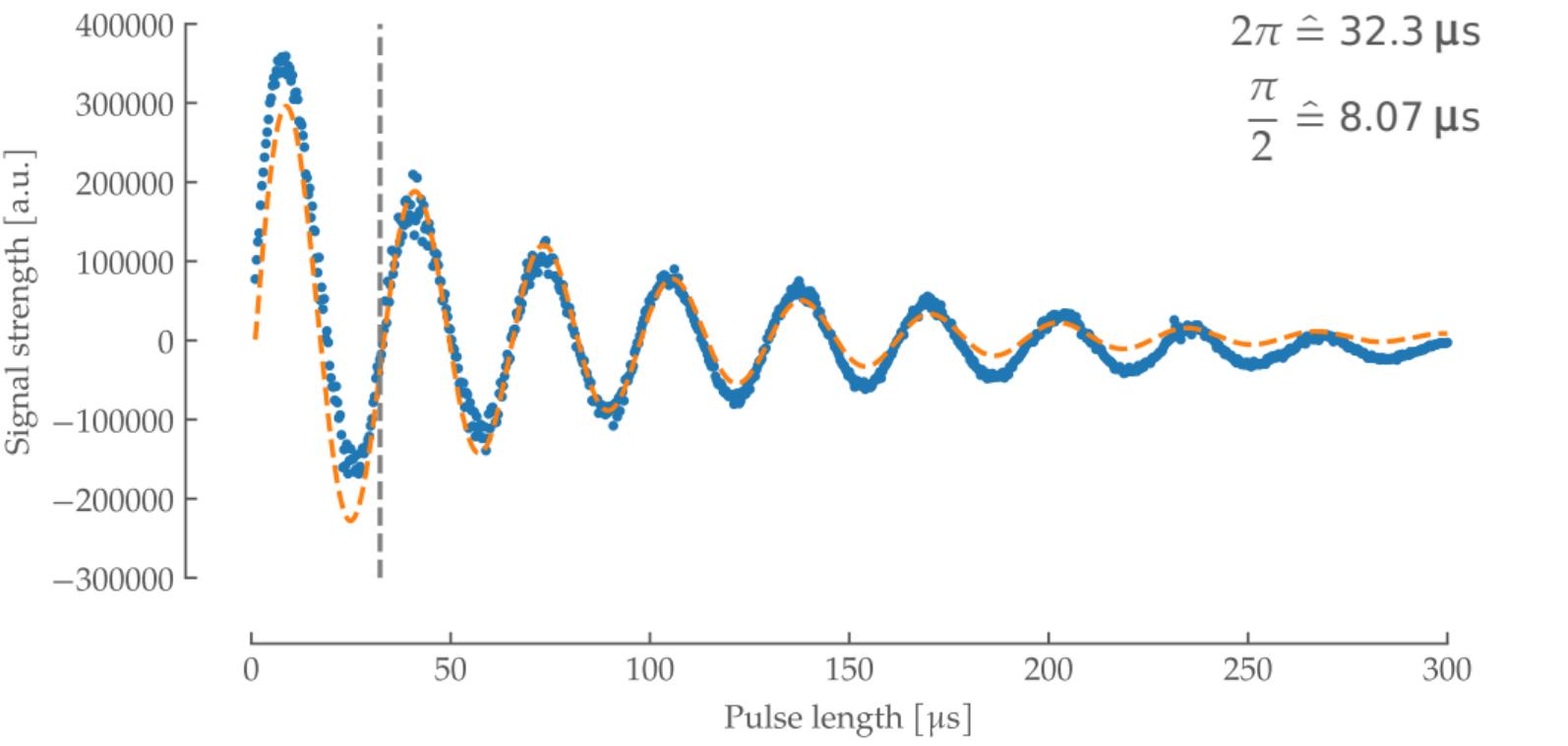
└ Experimental Results

It's a full tube of toluene, not a solution

1. Reasons for sidepeak: no apodization (truncation of FID), no shimming, inhomogeneities/not centred



Rabi nutation (pulse calibration) of water

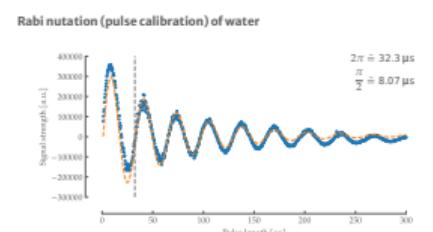


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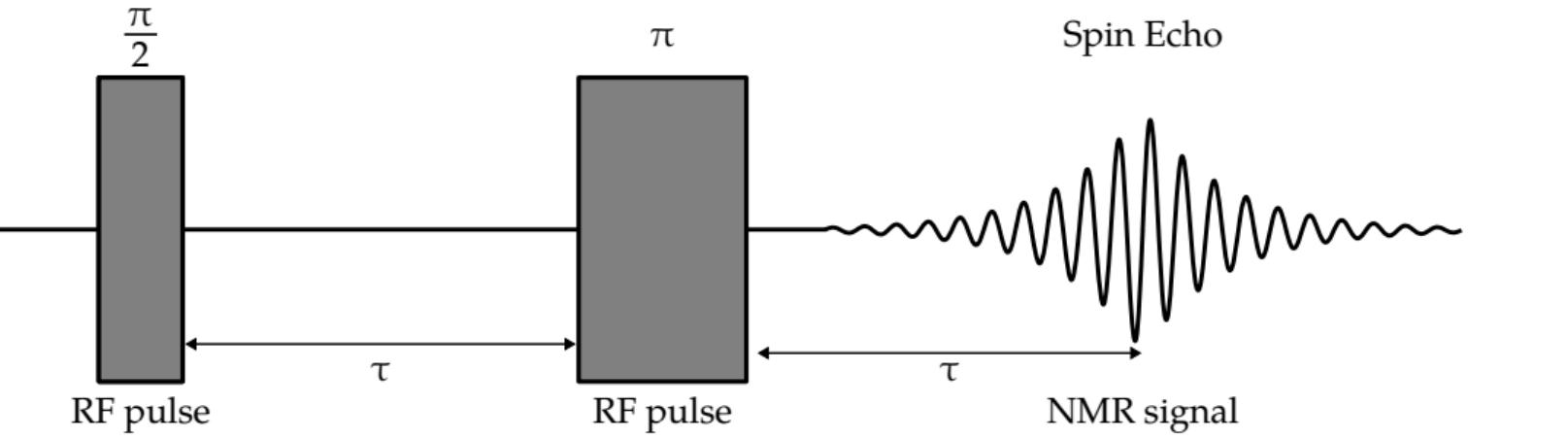
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└ Experimental Results

1. $T_{\text{period}} = 32 \mu\text{s}$
2. $T_{\frac{\pi}{2}} = 8 \mu\text{s}$



Spin Echo Sequence

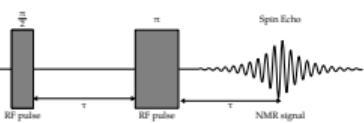


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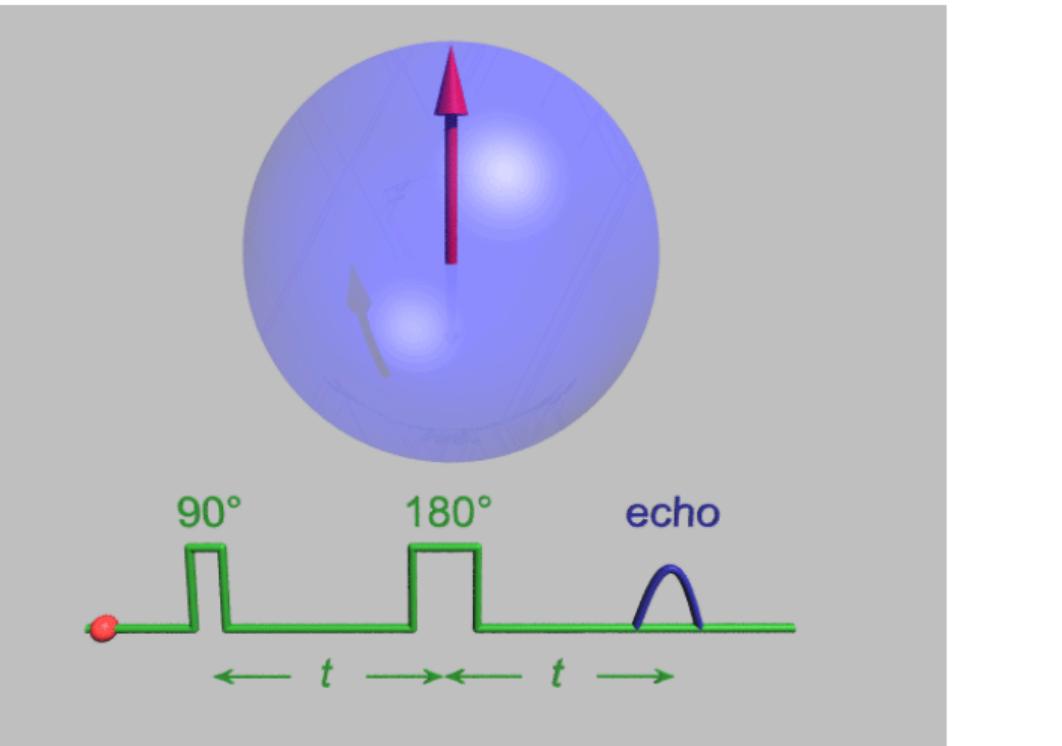
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└ Experimental Results

Spin Echo Sequence



Spin Echo Animation



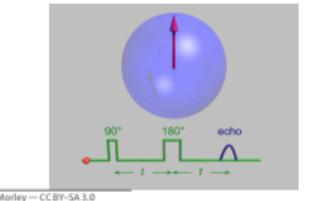
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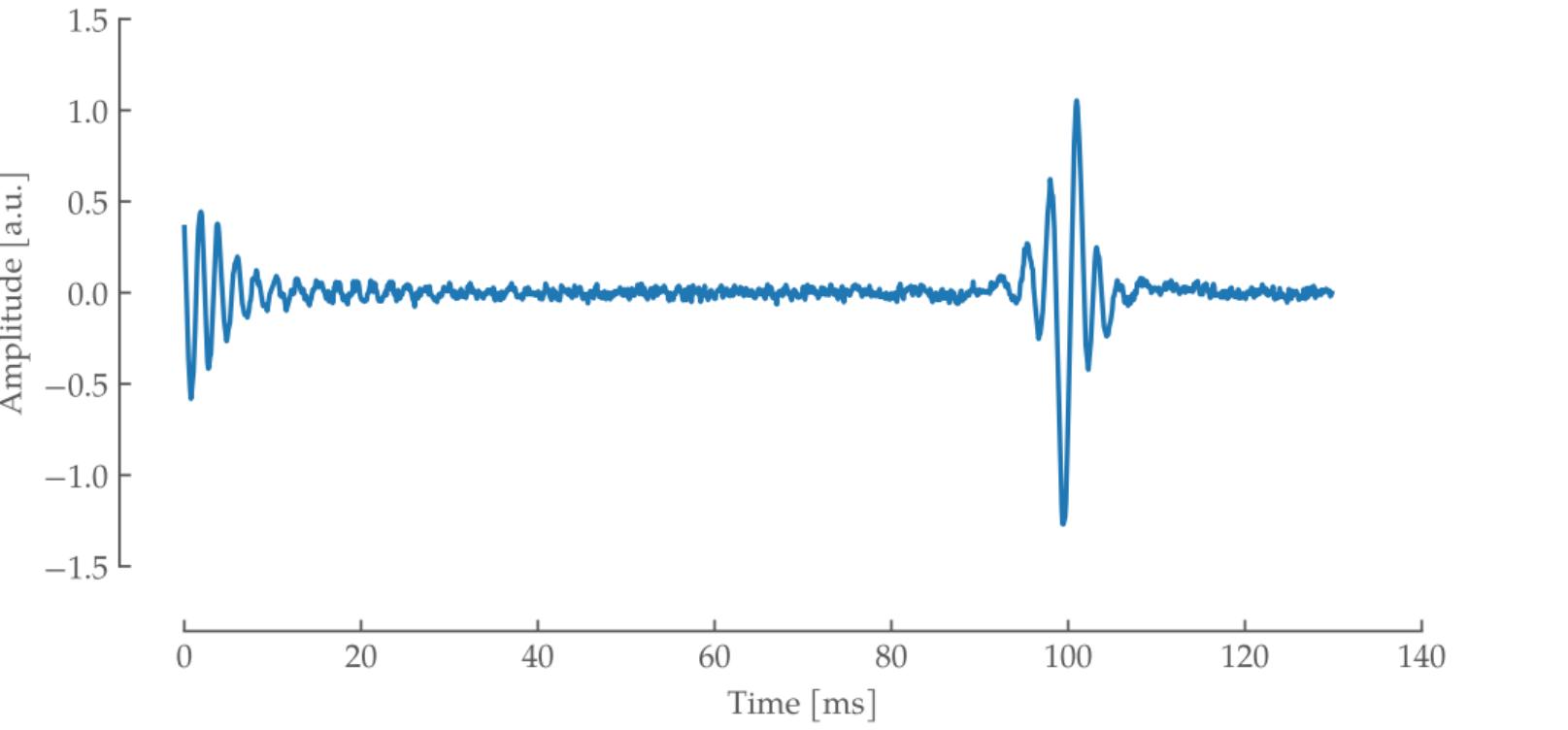
└ Experimental Results

Spin Echo Animation



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Spin Echo Measurement

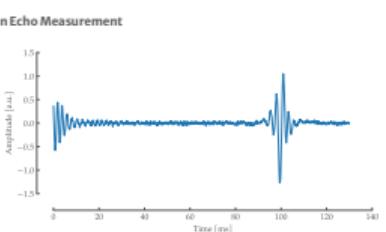


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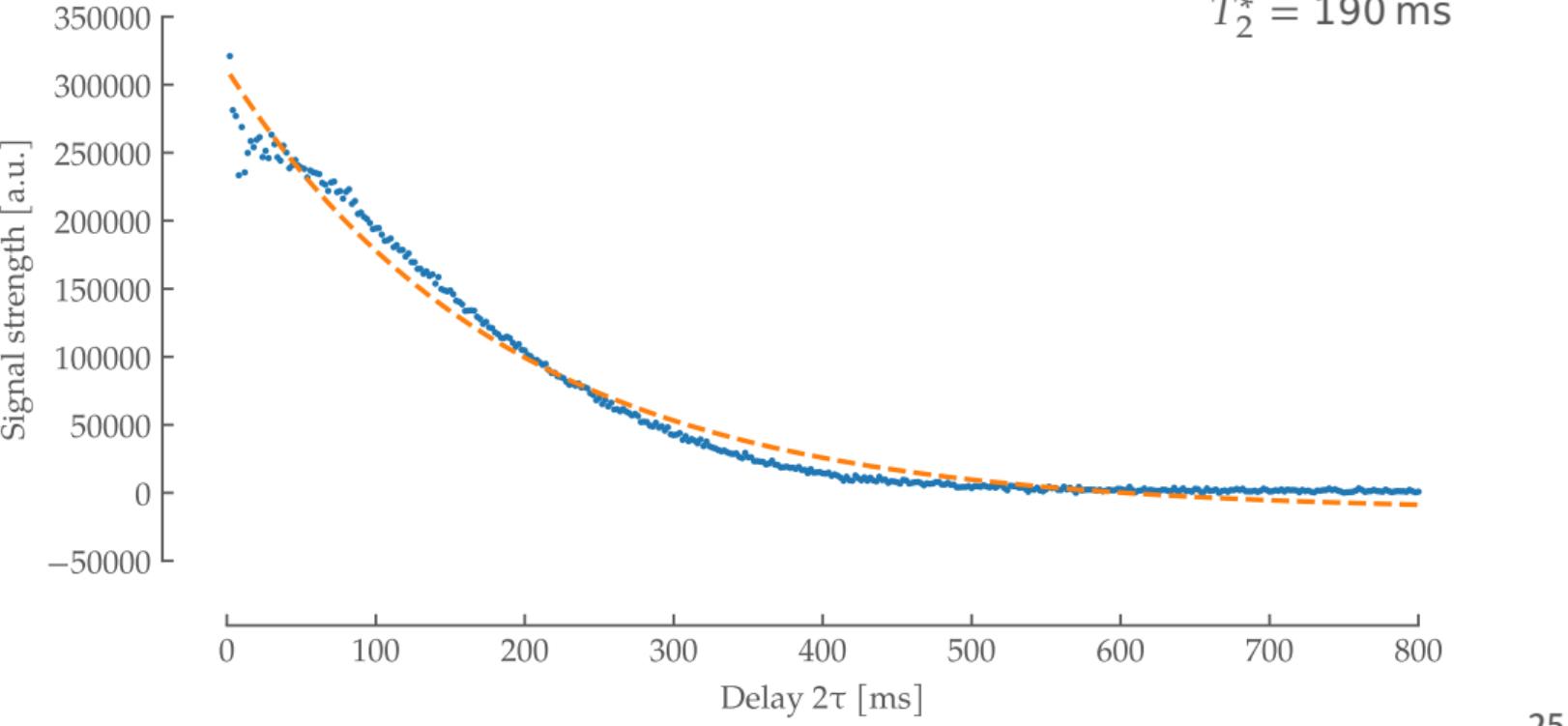
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└ Experimental Results



T_2 decay of water



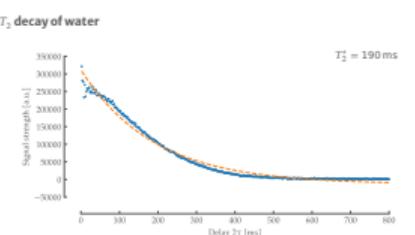
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└ Experimental Results

1. $T_2 =$



Demo time!

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└ Experimental Results

Review

- Why?
- The parts
 - Console
 - Amplifiers
 - Switch
 - Probe

- Capture & Process Software
- Experimental Results
- Demonstration

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└ Experimental Results

- Why?
- The parts
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Outlook

- Shim Driver
- Shielding
- Improve any part individually
 - Cheaper Magnet
 - Better Probe
 - Software (CIC compensation filter, frequency adjustment during pulse, ...)
- Investigate temperature stability
- Sell it to NexMR (or do Photo-CIDNP ourselves)

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Experimental Results

Outlook

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“I have not yet lost that sense of wonder, and of delight, that this delicate motion should reside in all ordinary things around us, revealing itself only to him who looks for it.”

“There the snow lay around my doorstep — great heaps of protons quietly precessing in the Earth’s magnetic field.”

— E.M. Purcell

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└ Experimental Results

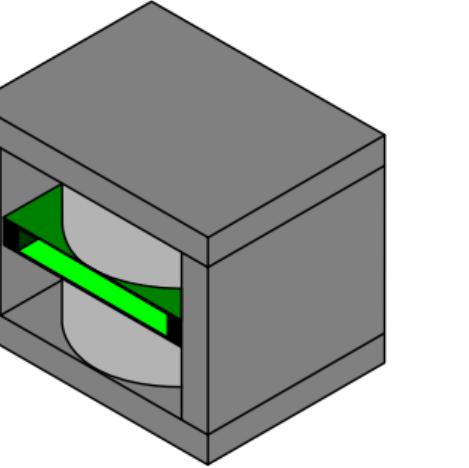
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— E.M. Purcell

1. Circling back to the beginning, I would like to end with a quote by E.M. Purcell
2. I wouldn’t have thought I would get a glimpse of this wonder that Purcell describes when starting my thesis here, but I’m glad I did.
3. And I hope none of you have lost it yet

Thank you!



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[https://gitlab.ethz.ch/mstabel/
nmr-spectrometer](https://gitlab.ethz.ch/mstabel/nmr-spectrometer)



Find everything on

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└ Experimental Results

Thank you!

Find everything on



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nmr-spectrometer](https://gitlab.ethz.ch/mstabel/nmr-spectrometer)



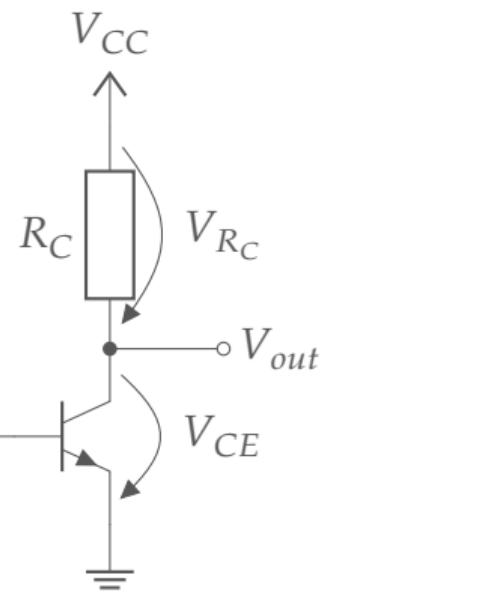
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Backup

An amplifier is basically just a transistor

- Transistor:
voltage-controlled current source
- higher voltage → higher current
 - higher voltage V_{R_C}
 - lower voltage V_{CE}
 - 180° phase shift

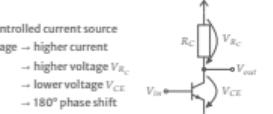


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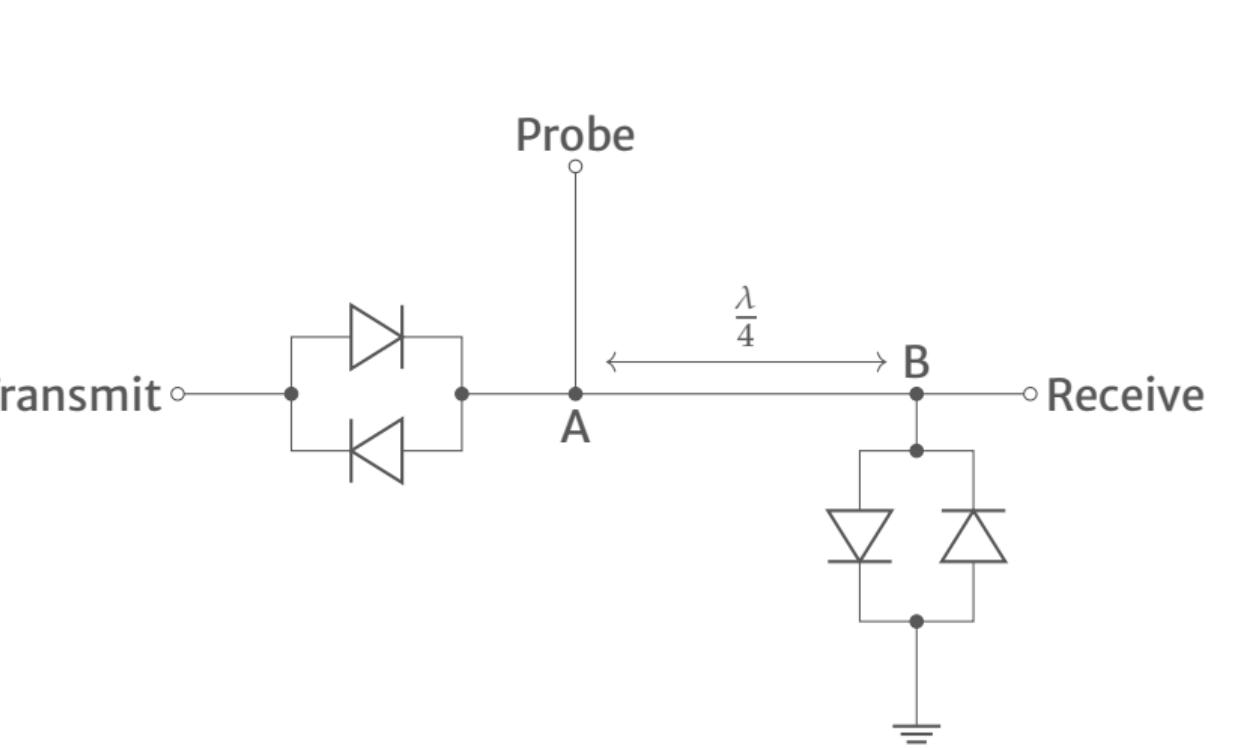
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└ An amplifier is basically just a transistor

1. We want cheap, so using a simple is the obvious first approach
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 - Input/Output Impedance Matching
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 - stability calculations
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The passive approach leaked too much power

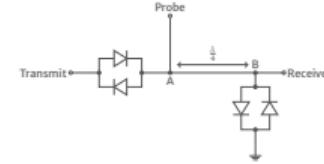


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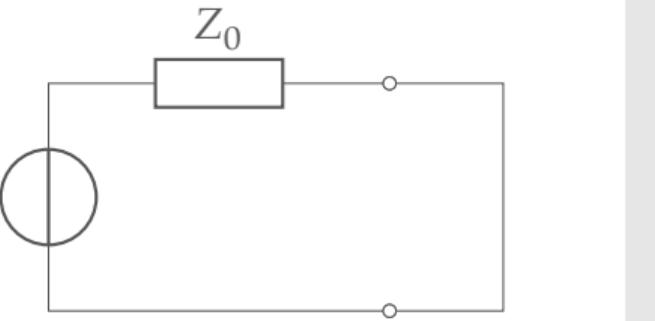
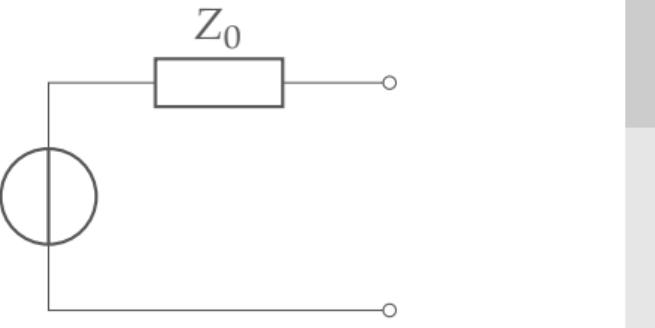
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└ The passive approach leaked too much power

1. So called "video feedthrough"
2. Especially noise during reception phase, leaking through turned off amplifier
3. "Traditional" passive design by Lowe and Tarr
4. Leads to distortion of low-power pulses
5. Same design can be used with PIN-Diodes (effectively current-controlled resistor)
6. But PIN Diodes often need higher frequencies (mid MHz), size of intrinsic semiconductor



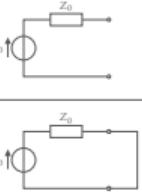
A transmission line transforms impedance



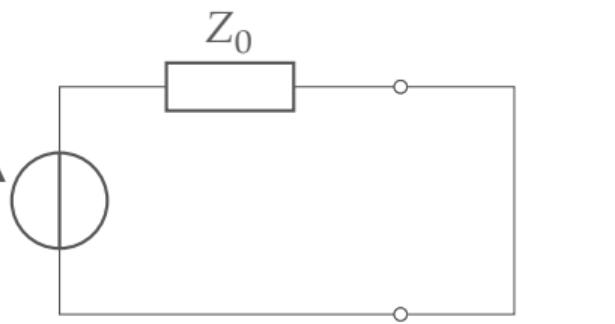
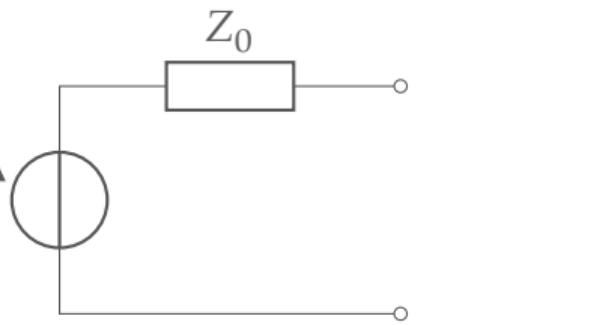
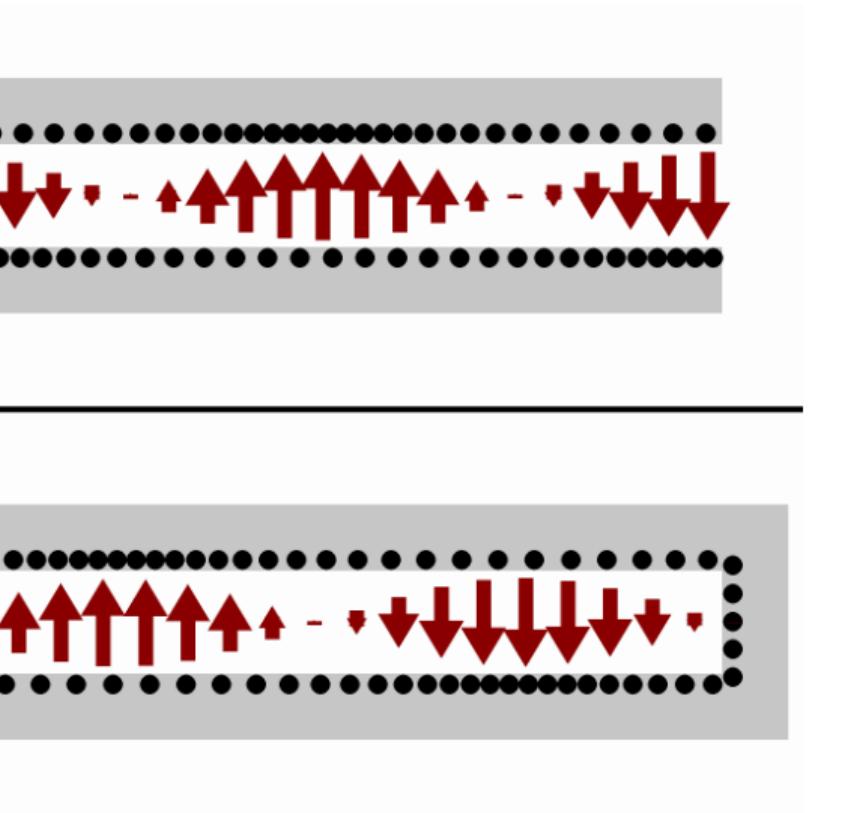
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└ A transmission line transforms impedance



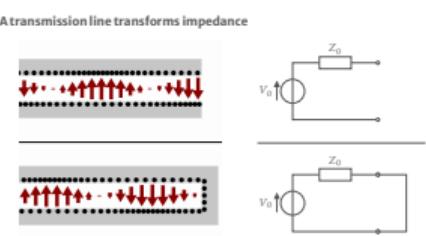
A transmission line transforms impedance



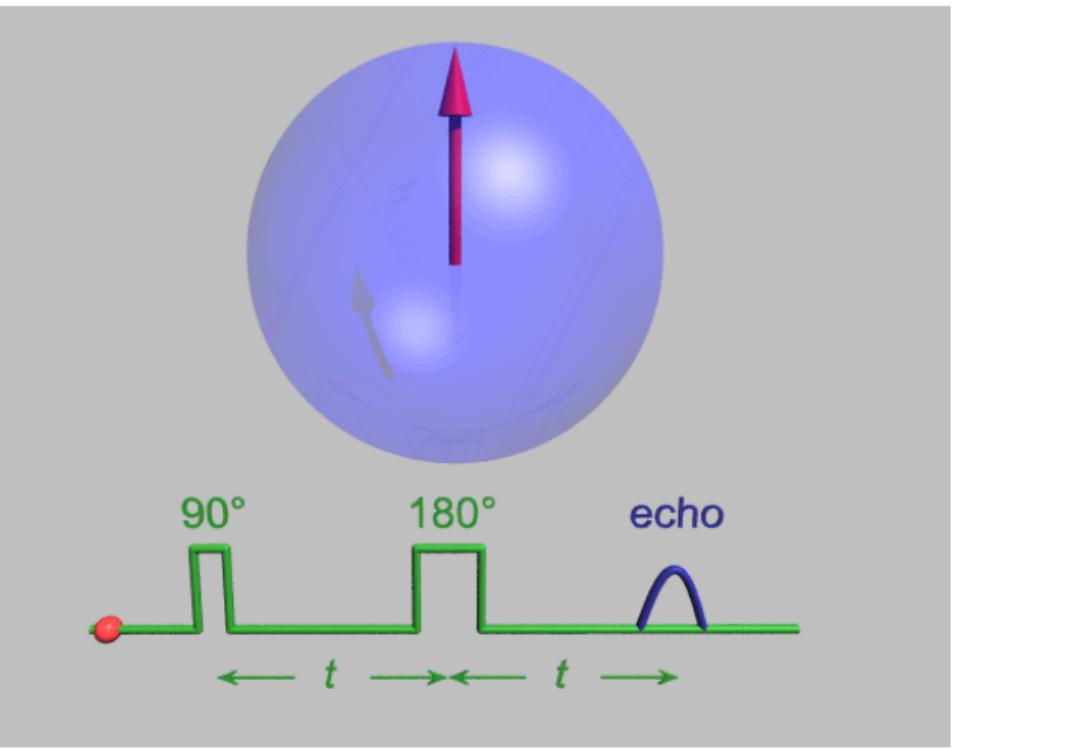
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└ A transmission line transforms impedance



T_2 Decay Animation



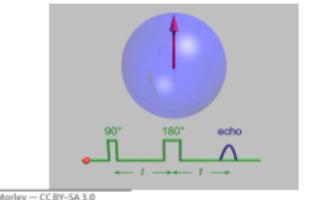
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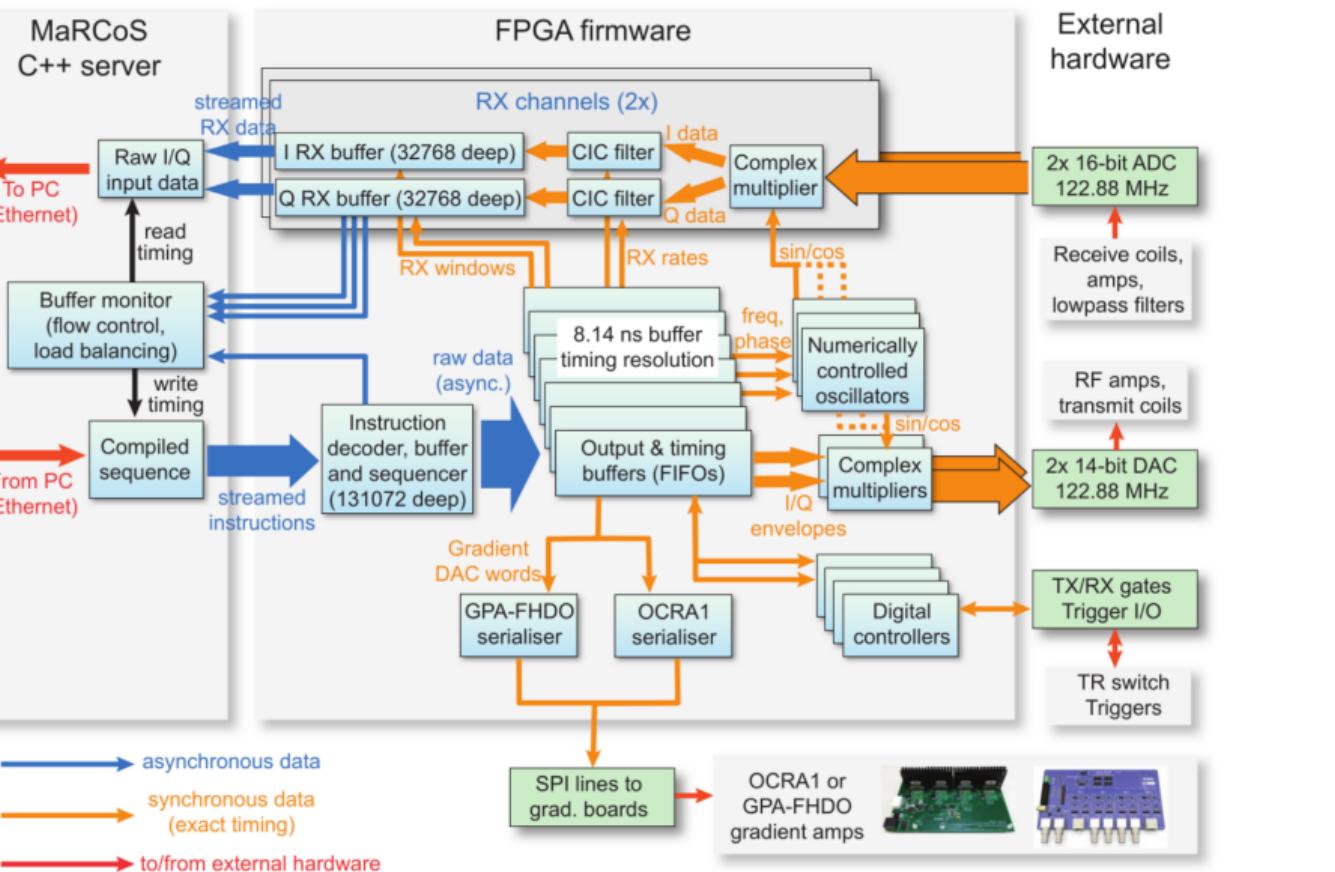
magnETHical

└ T_2 Decay Animation

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