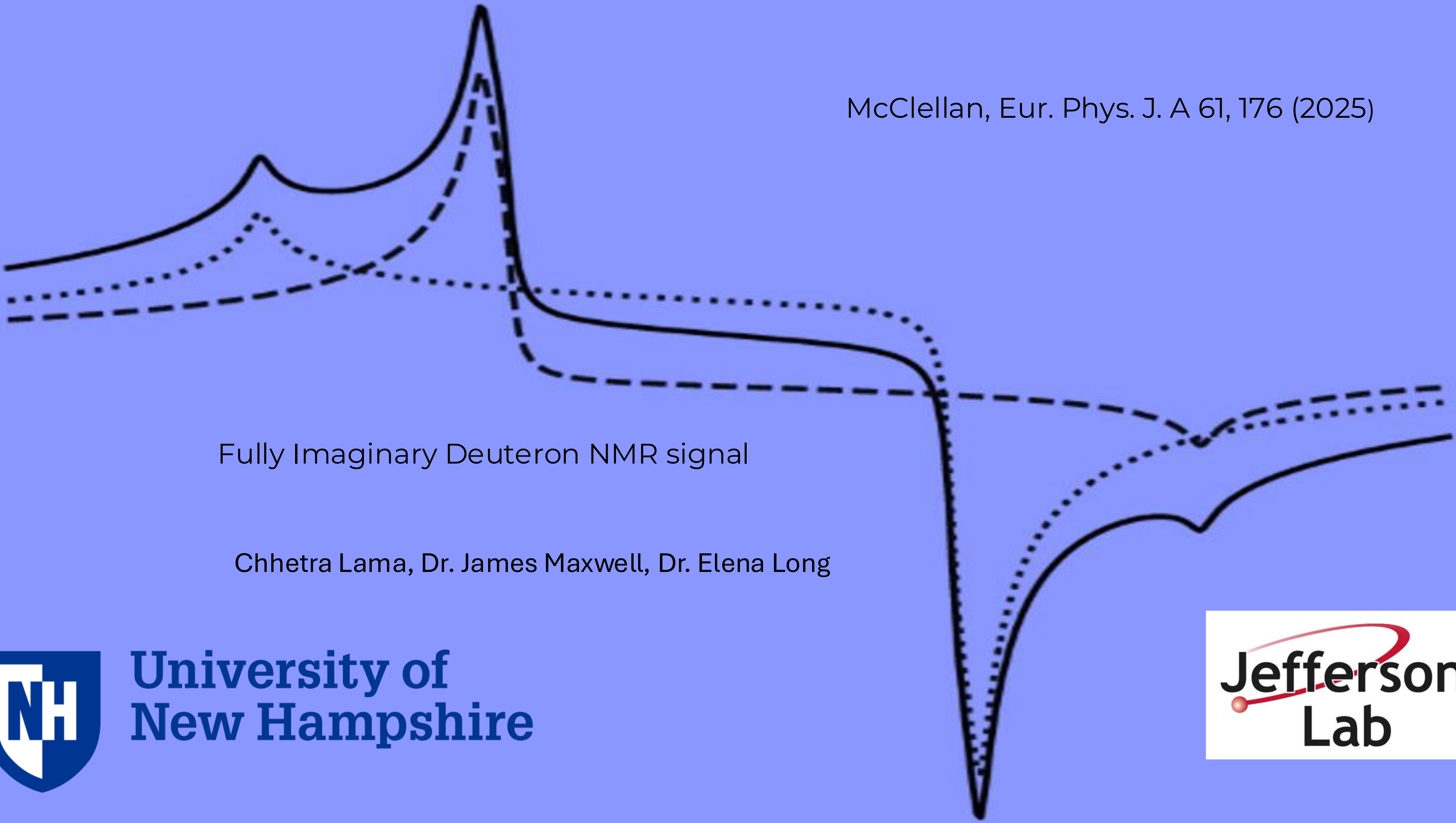

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Fully Imaginary Deuteron NMR signal

Chhetra Lama, Dr. James Maxwell, Dr. Elena Long

University of New Hampshire

Jefferson Lab

Fully Imaginary Signal Implementation to the Jlab Q-meter

Add the imaginary deuteron signal and phase angle to the JLab Q-meter software to help reduce systematic uncertainties in the NMR measurements.

"Complex NMR signal"

Built on code originally written by James Maxwell and used during the first Run Group C run.

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Acknowledgement

DOE Award DE-FG02-88ER40410

C12-13-011: The b_1 *experiment*

30 Days in Jlab Hall C
A- Physics Rating

C12-15-005: A_{zz} *for x>1*

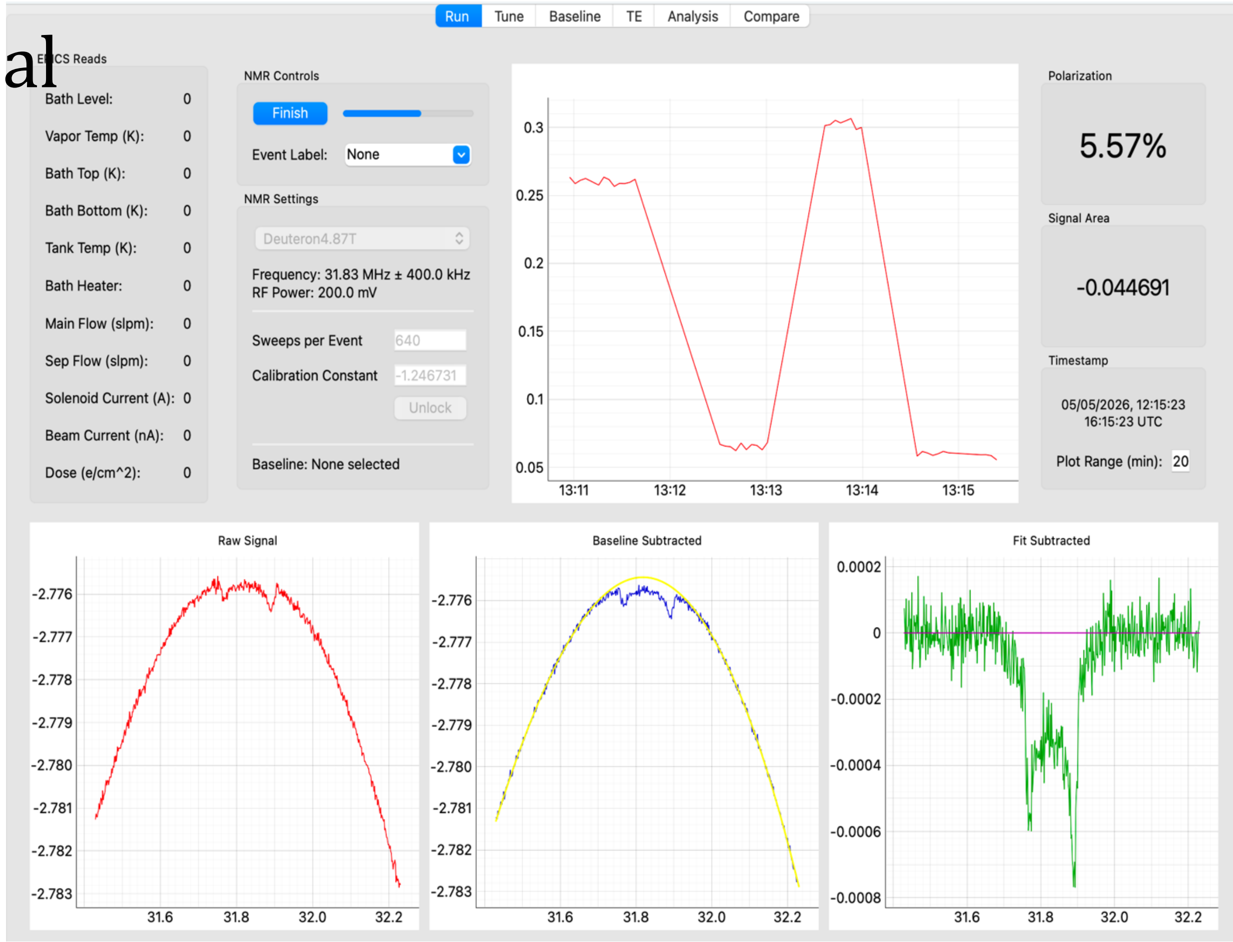
44 Days in Jlab Hall C
A- Physics Rating

Run Group Spokespersons

Chen, Day, Higinbotham, Keller
Long, Rondon, Slifer, Solvignon

Outline

- ➢Motivation for Complex Deuteron Signal
- ➢Theoretical Concept of Prior Fit
- ➢Fitting Principle of Complex Signal
- ➢Modified Example Results
- ➢Conclusion



James Software

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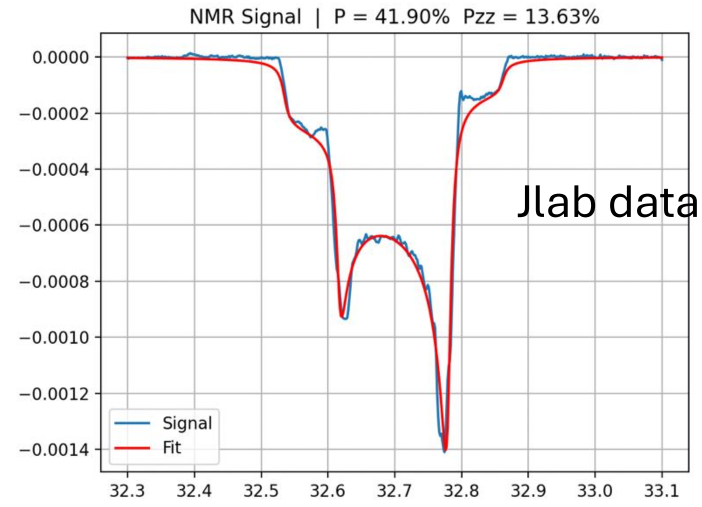
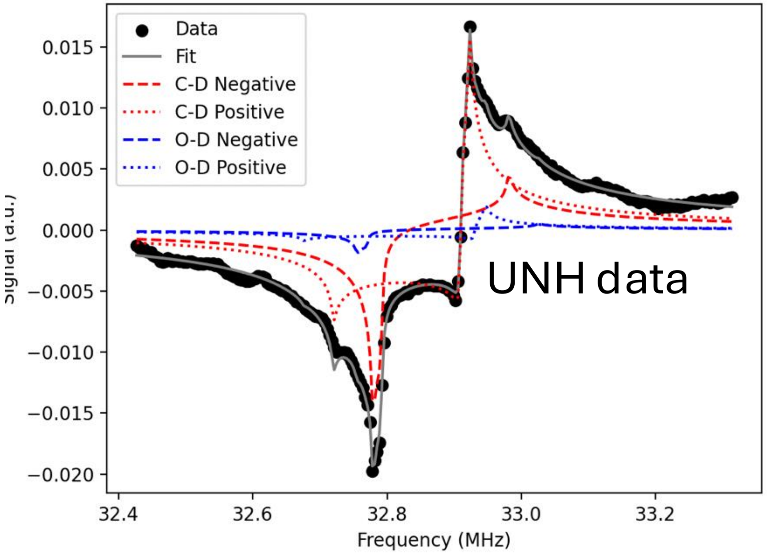
Motivation

❖Goal: Get more accurate value of Polarization; reduce systematic uncertainties, tackle off-phase signal





❖Current Status:

✓Absorptive and dispersive both function are used to analyze the signal

✓ False asymmetry and scaling both version are used to analyze the Polarization

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Motivation continued

The correct way to determine the asymmetry, r, is by fitting the equation of the absorption function from this theory to NMR signals, not by dividing the peak heights. Then the polarization can be calculated from Eq. (20). Using Eqs. (14, 15, 21, 22) the absorption function for large quadrupole broadening reads

$$\chi''(r,R) \propto \left(\frac{1}{\omega_q}\right)\left\{\left[\frac{r^2 - r^{1-3\vartheta R}}{r^{1-\vartheta R}}\right] F_+(R) + \left[\frac{r^{1+3\vartheta R} - 1}{r^{1+\vartheta R}}\right] F_-(R)\right\}, \quad (24)$$

while for deuterated butanol material in a 2.5 T field, where $\vartheta \gg 1$, the absorption function in good approximation is

$$\chi''(r,R) \propto \left(\frac{1}{\omega_q}\right)\left(\frac{r-1}{r}\right)[rF_+(R) + F_-(R)]. \quad (25)$$

3.2. *False asymmetry and false polarization*

The Q-meter distortions appear as a false asymmetry in the deuteron TE signal. It manifests itself by increasing the size of the right side of the signal by a few percent with respect to the left side. Since the TE signal has a small and well-known asymmetry which results from its $P_{TE} = 0.0523\,\%$ polarization, it provides a very clean way to measure this asymmetry and therefore it enables the parameterization of the effects of the Q-meter distortions.

A more exact relation [17] for Eq. (3) is available and can be used to estimate higher-order frequency-dependent corrections to the NMR signal defined in Eq. (27). A detailed example calculation of this distortion can be found in Ref. [18] which shows that a small mixing of χ' into the signal causes this effect. The distortion is approximated well be a linear gain across the deuteron signal which can be summarized by

$$D(\omega) = 1 + \tfrac{1}{2}\xi(1+R), \quad (28)$$

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$$S(\omega) = c\chi''(\omega)[1 + \frac{1}{2}\xi R] \quad (19)$$

However, once the phase angle is included in curve-fitting, $\mathcal{P}$ and $\mathcal{Q}$ can be determined regardless of the phase angle. One can polarize target material while switching between different phase angles and still extract a consistent spin-up curve via the ratio method (Fig. 10), allowing one to observe patterns in both real and imaginary views of the signal during polarization. Even with exceptionally good tuning (a phase angle at or near 0°), it is still more correct to use the full complex form of the signal, as the signal is itself still complex.

$$\Xi = c(a\mathcal{P}^4 + b\mathcal{P}^2 + 1) \quad (20)$$

where c is the remaining constant portion of the scaling factor. This makes Eq. (18)

$$S(\omega) = \Xi[\chi''\cos(\theta) - \chi'\sin(\theta)] \quad (21)$$

By extension, Ξ is dependent on r via Eq. (13):

$$\Xi = c\left[a\left(\frac{r^2-1}{r^2+r+1}\right)^4 + b\left(\frac{r^2-1}{r^2+r+1}\right)^2 + 1\right] \quad (22)$$

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https://github.com/jdmax/jlab_py

Fitting Principle on Current Software

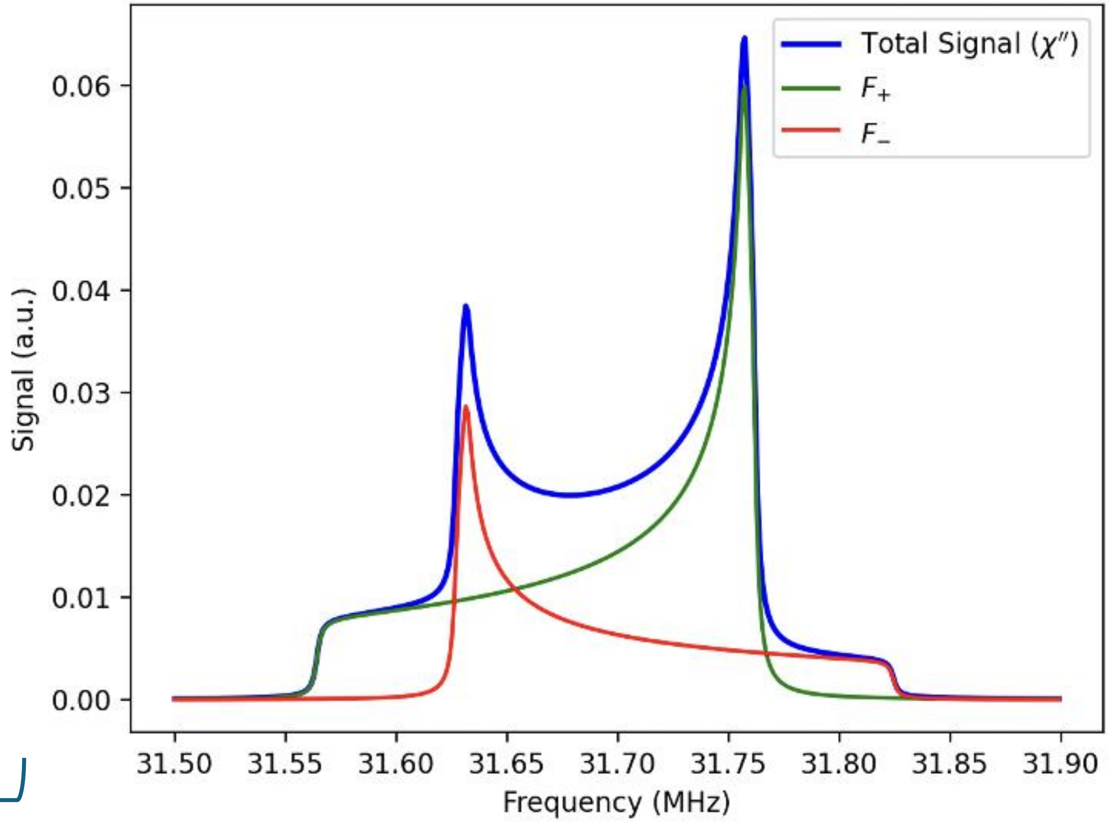
$$f_\in(R,A,\eta,\phi) = \frac{1}{2\pi\varrho}\left\{ \begin{array}{l} 2\cos\left(\frac{\alpha}{2}\right)\left[\arctan\left(\frac{Y^2-\varrho^2}{2Y\varrho\sin\left(\frac{\alpha}{2}\right)}\right)+\frac{\pi}{2}\right] \\ +\sin\left(\frac{\alpha}{2}\right)\ln\left(\frac{Y^2+\varrho^2+2Y\varrho\cos\left(\frac{\alpha}{2}\right)}{Y^2+\varrho^2-2Y\varrho\cos\left(\frac{\alpha}{2}\right)}\right) \end{array} \right\}$$

$$F_\varepsilon(R,A,\eta) = \frac{1}{J+1}\sum_{j=0}^{J}\frac{\sqrt{3}\,f_\in(R,A,\eta,\phi)}{\sqrt{3-\eta\cos(2\phi)}}$$

Spin flips

$$\chi''(r,R) \propto (1/\omega_q)\left\{\left[\frac{r^2-r^{1-3\vartheta R}}{r^{1-\vartheta R}}\right]F_+(R) + \left[\frac{r^{1-3\vartheta R}-1}{r^{1+\vartheta R}}\right]F_-(R)\right.$$

F_+ F_-



$$D(\omega) = 1 + \frac{1}{2}\xi(1+R)$$

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https://github.com/jdmax/jlab_pynmr

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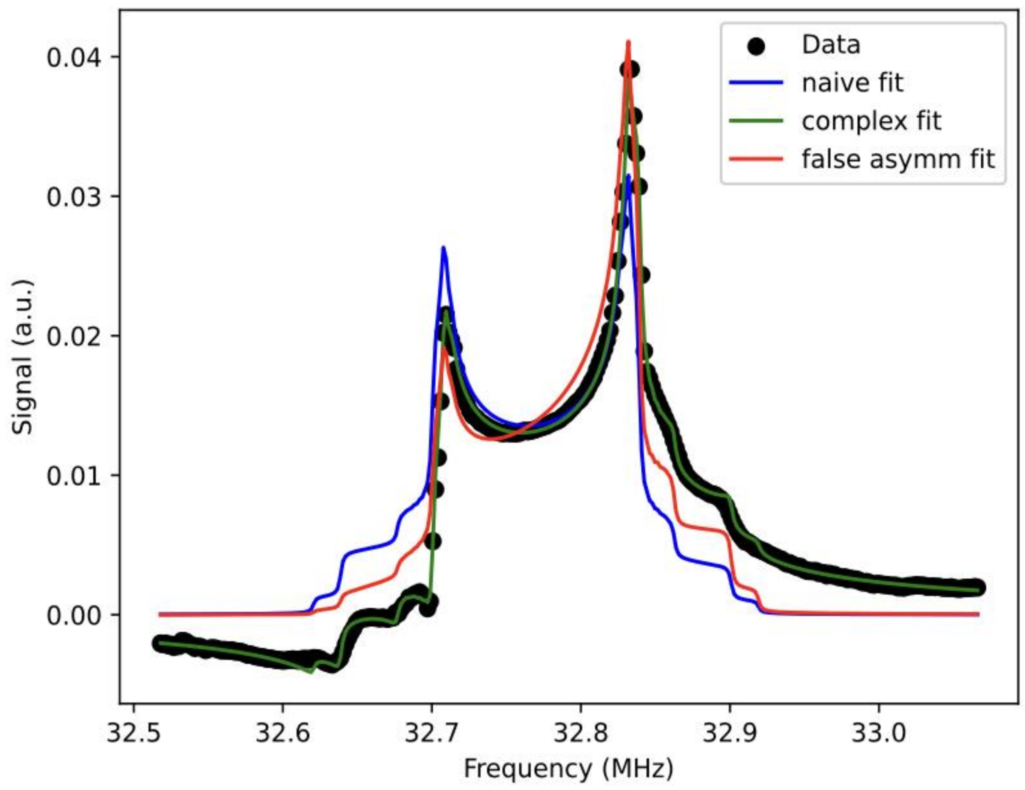
Upgrading to Complex Fit

$$f'_{\epsilon}(R, A, \eta, \phi) = \frac{1}{2\pi\varrho}\left\{ 2\sin\left(\frac{\alpha}{2}\right)\left[\arctan\left(\frac{Y^2-\varrho^2}{2Y\varrho\sin\left(\frac{\alpha}{2}\right)}\right)+\frac{\pi}{2}\right] + \cos\left(\frac{\alpha}{2}\right)\ln\left(\frac{Y^2+\varrho^2+2Y\varrho\cos\left(\frac{\alpha}{2}\right)}{Y^2+\varrho^2-2Y\varrho\cos\left(\frac{\alpha}{2}\right)}\right)\right\}$$

False asymmetry term is removed with Ξ

$$\Xi = c\left(a\left(\frac{r^2-1}{r^2+r+1}\right)+b\left(\frac{r^2-1}{r^2+r+1}\right)+1\right)$$



$$F_{complex} = Scale * \Xi\left(F_{absorptive} * \cos(phase) + F_{dispersive} * \sin(phase)\right)$$

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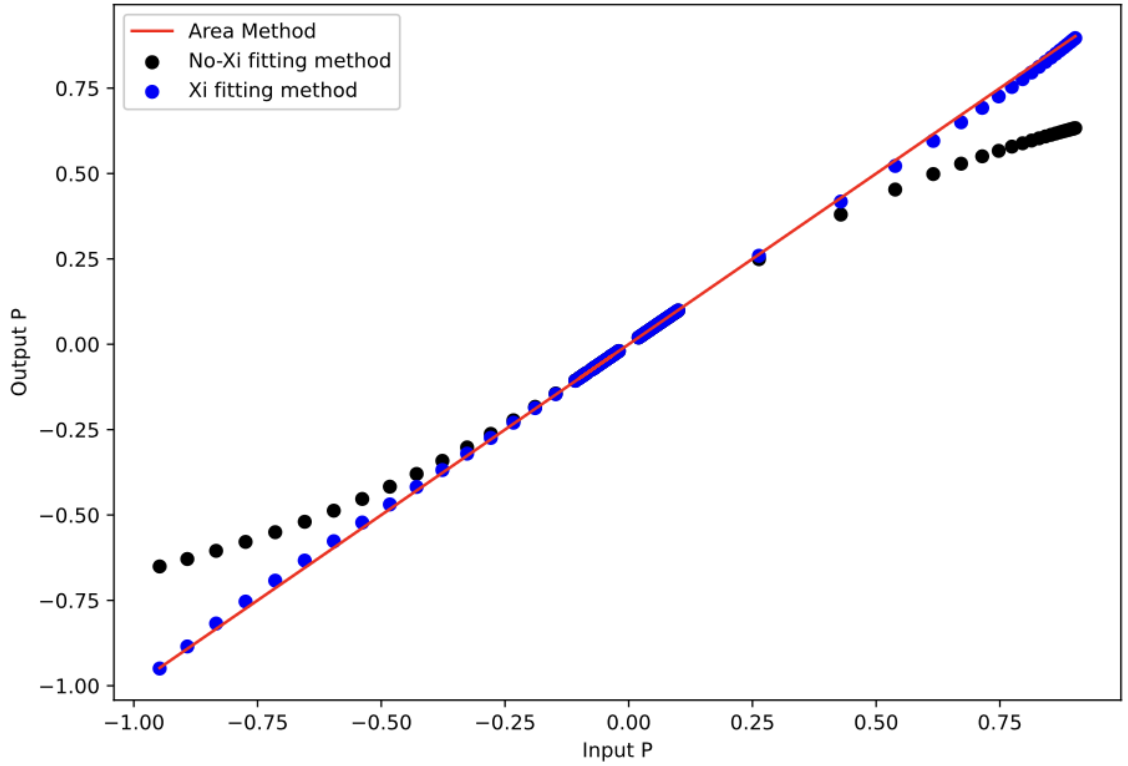
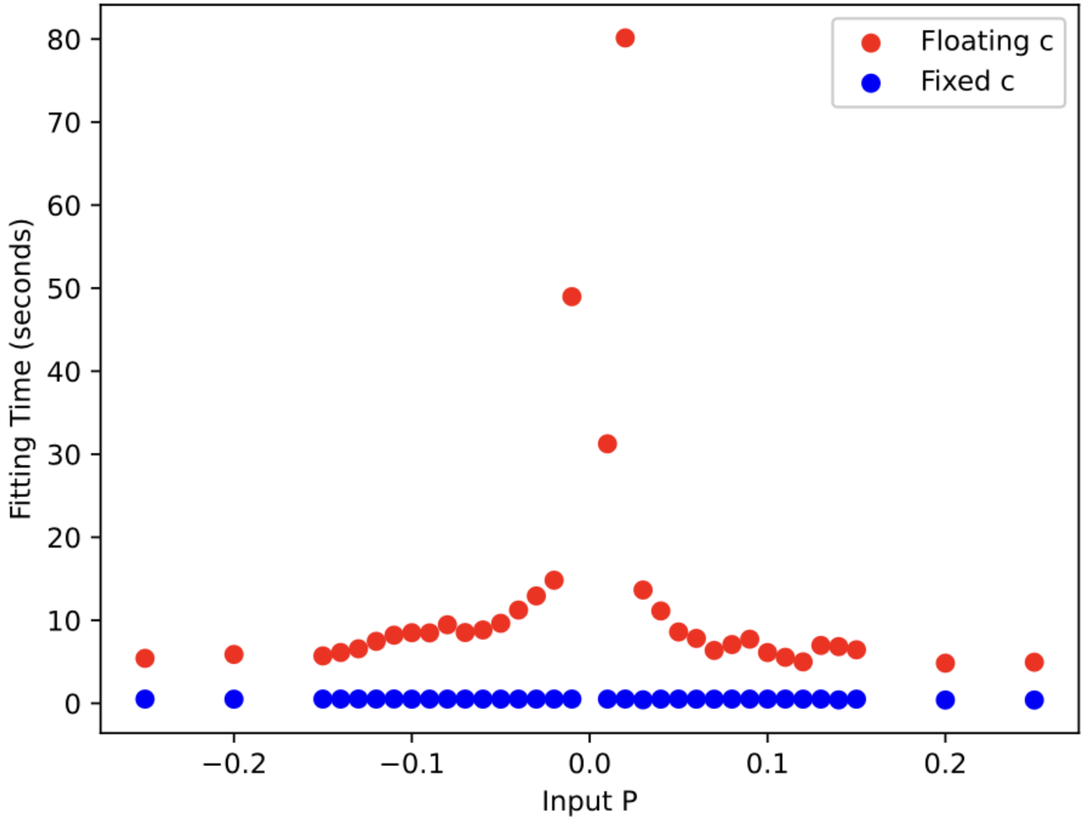
Why Ξ(xi)?



More accurate over all range of P



Quicker Computation Time

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https://github.com/jdmax/jlab_pynmr

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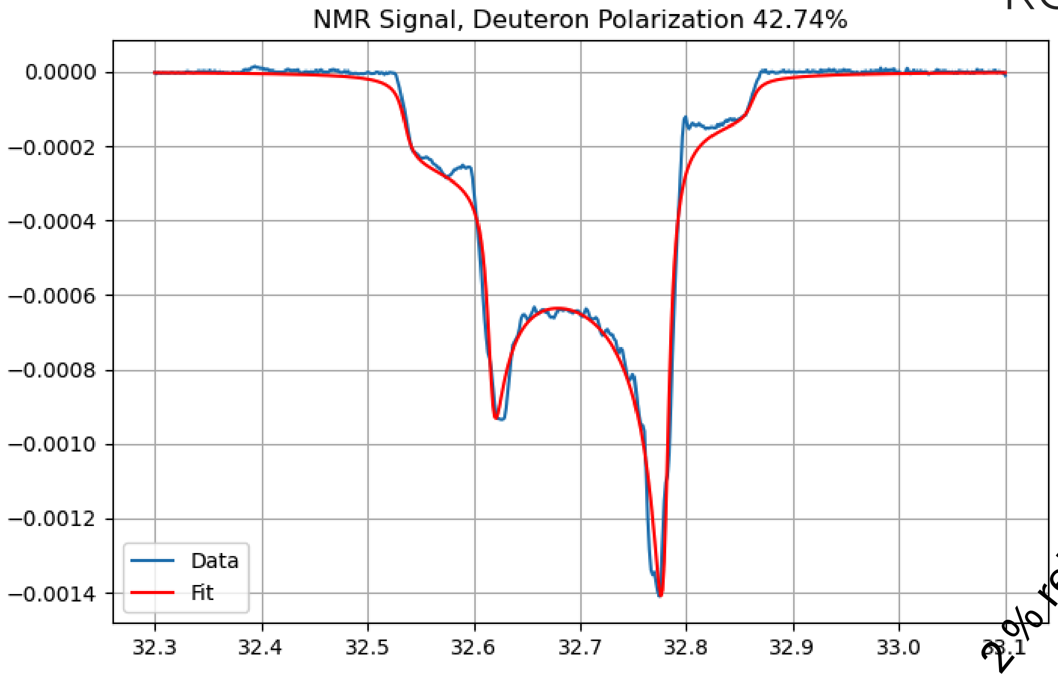
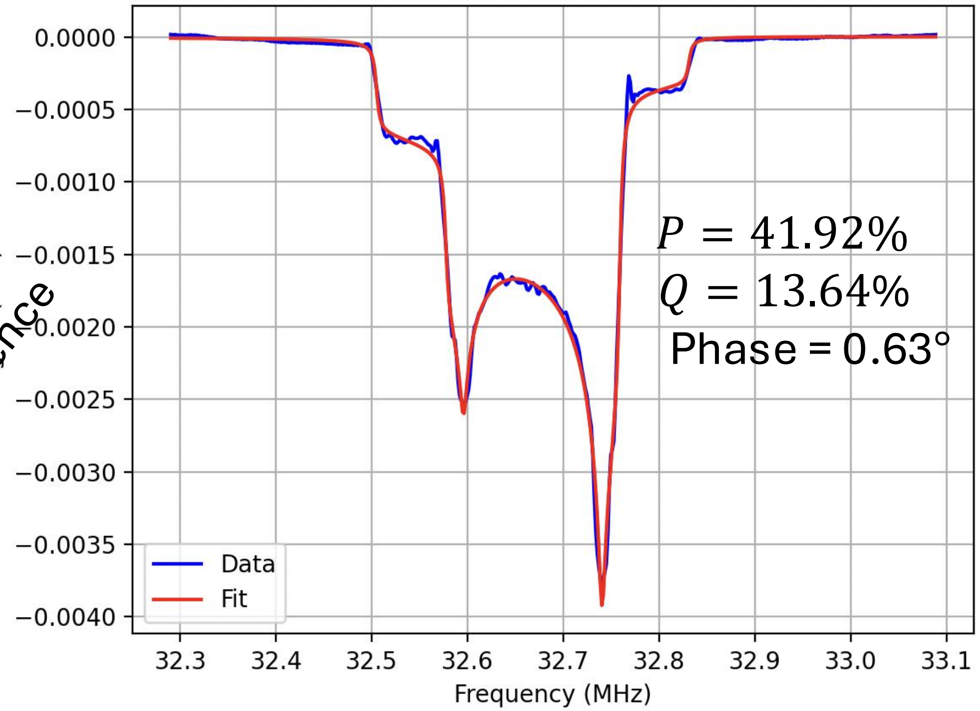
Fit with and w/o dispersive function

RGC 2022 data



2% relative difference



w/o dispersive function

With dispersive function

RGC E12-06-109 Spokespersons

Crabb, Deur, Dharmawardane, Forest, Griffioen, Holtrop, Kuhn, Prok

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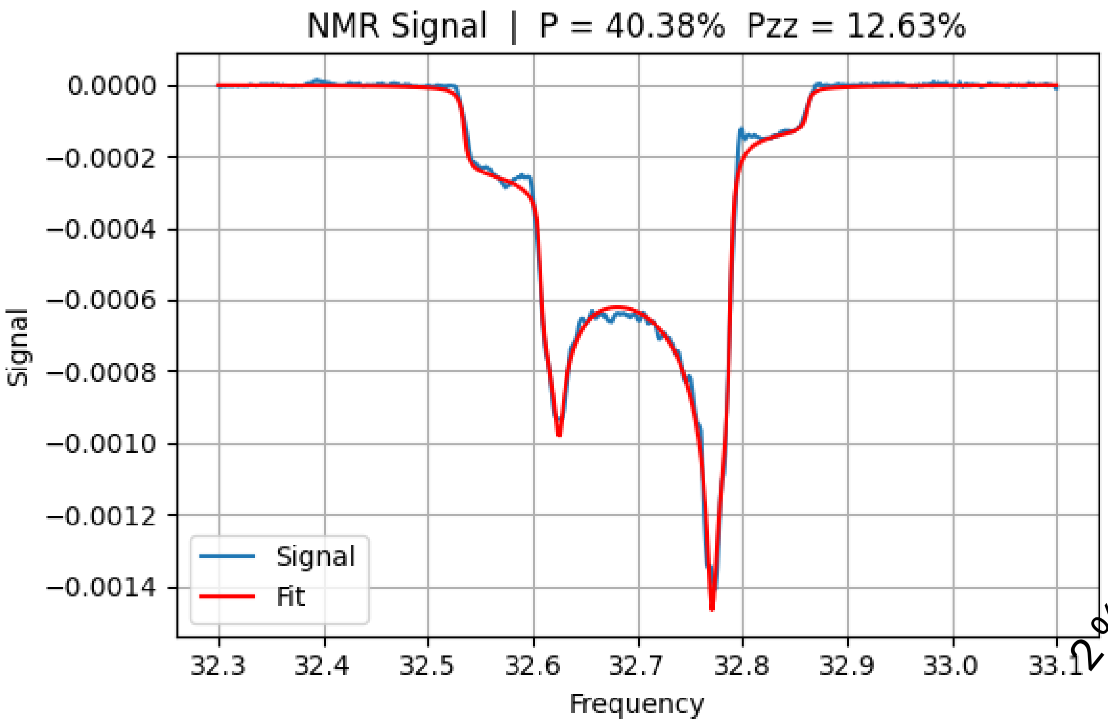
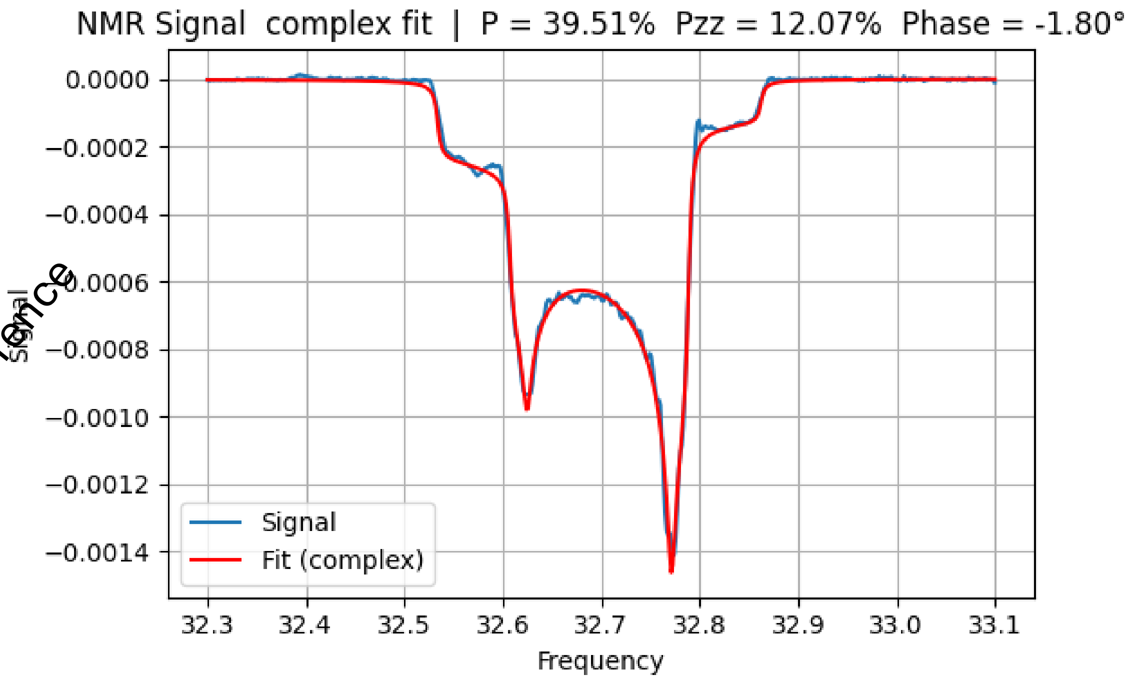
Fit with and w/o dispersive function continued

RGC 2022 data



w/o dispersive function

2 % relative difference



With dispersive function

https://github.com/jdmax/DeuteronPeakFit/blob/master/example.ipynb

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https://github.com/jdmax/jlab_pynmr

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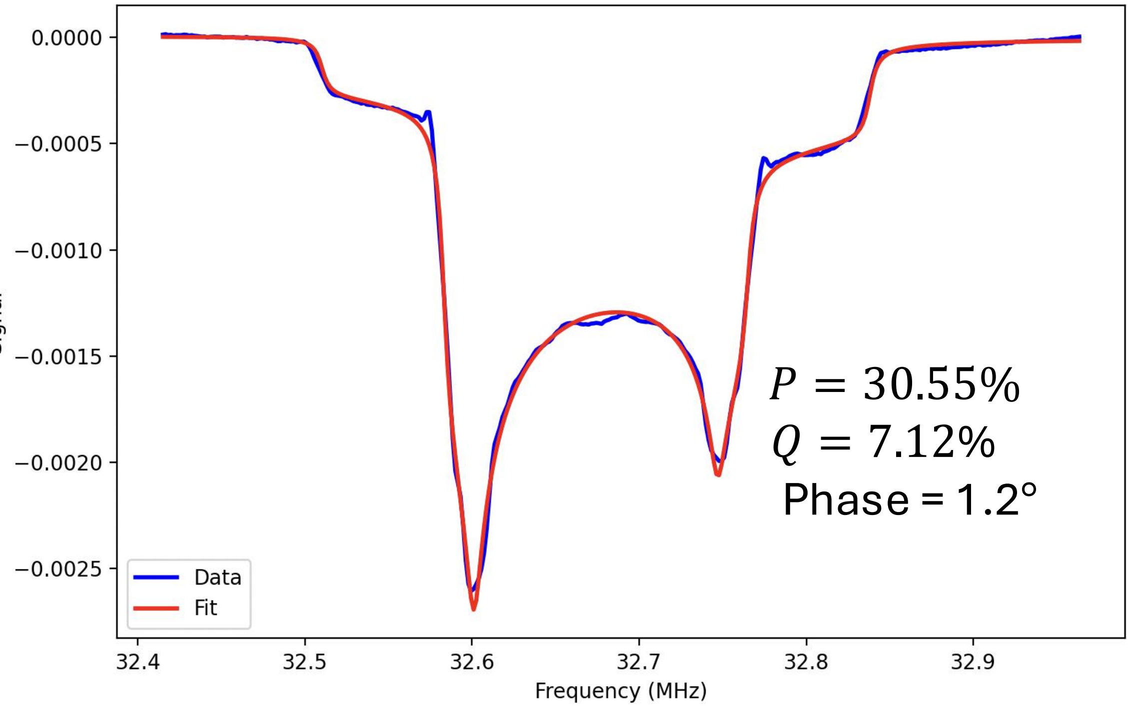
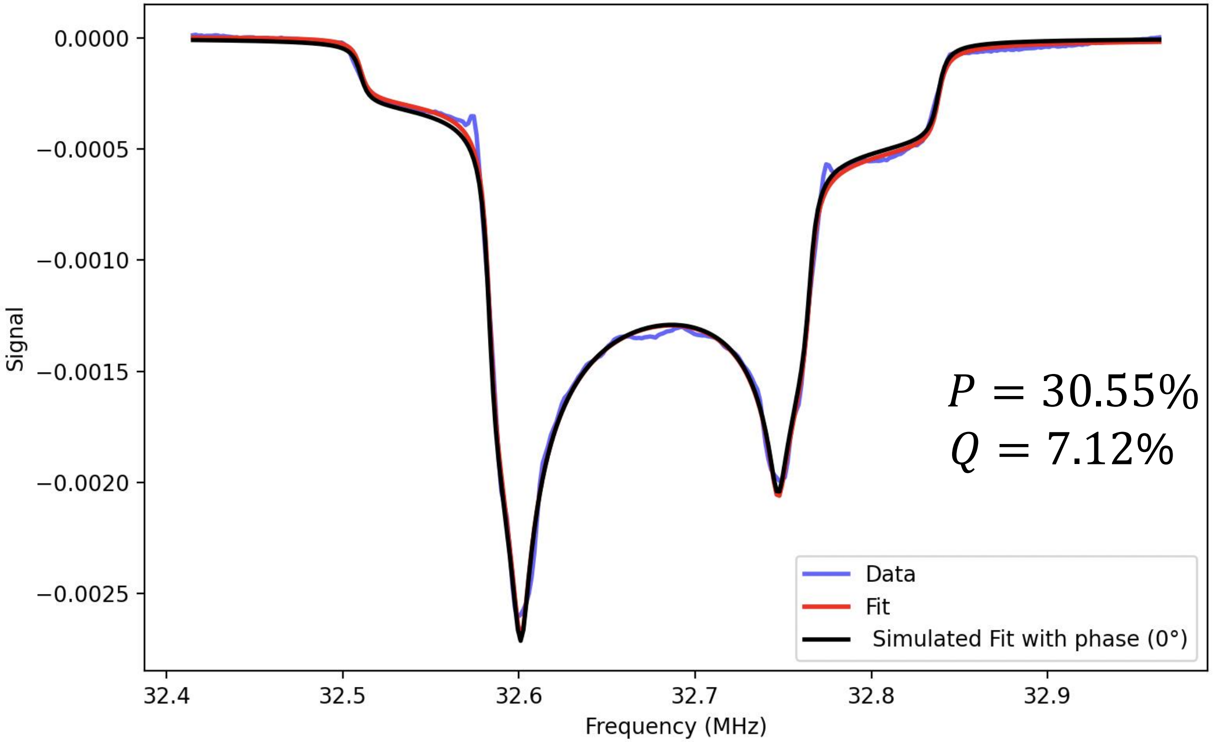
What will happen if we have mixed phase(Simulation)

RGC 2022 data



Data with Fit



Data with Fit and simulated phase

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https://github.com/jdmax/jlab_pynmr

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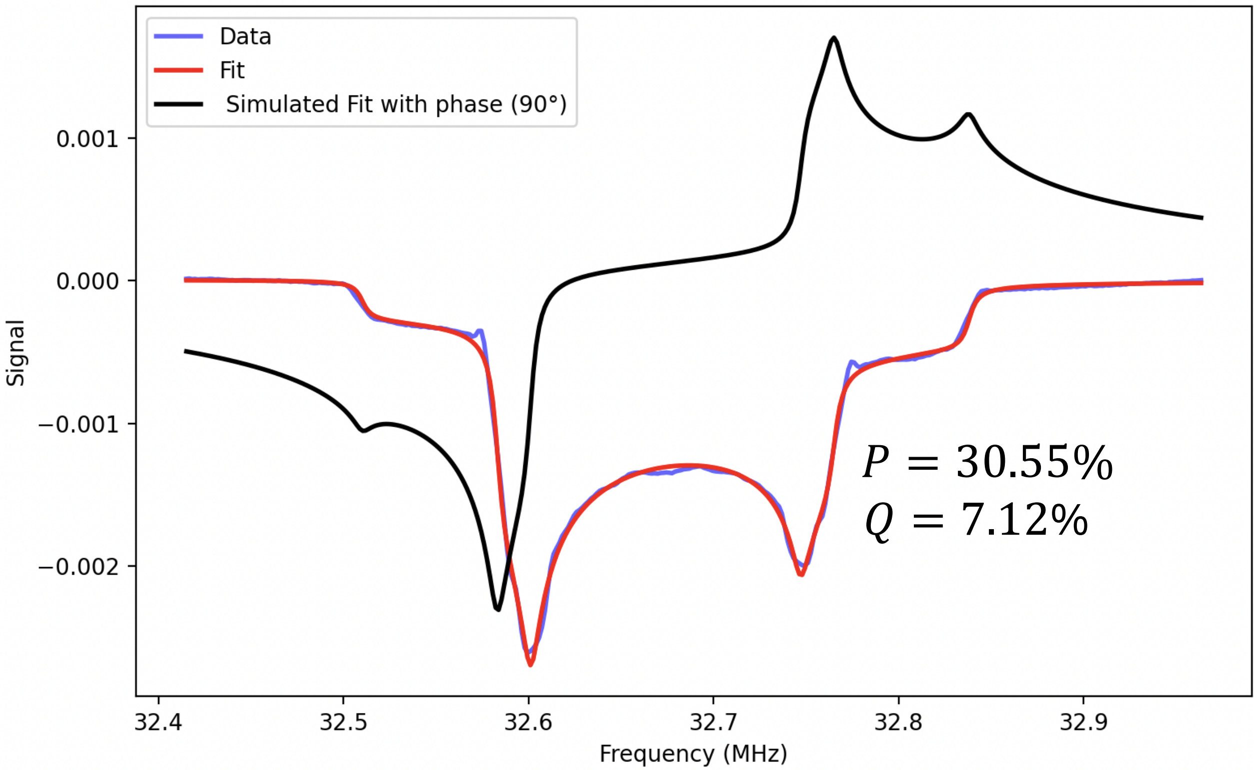
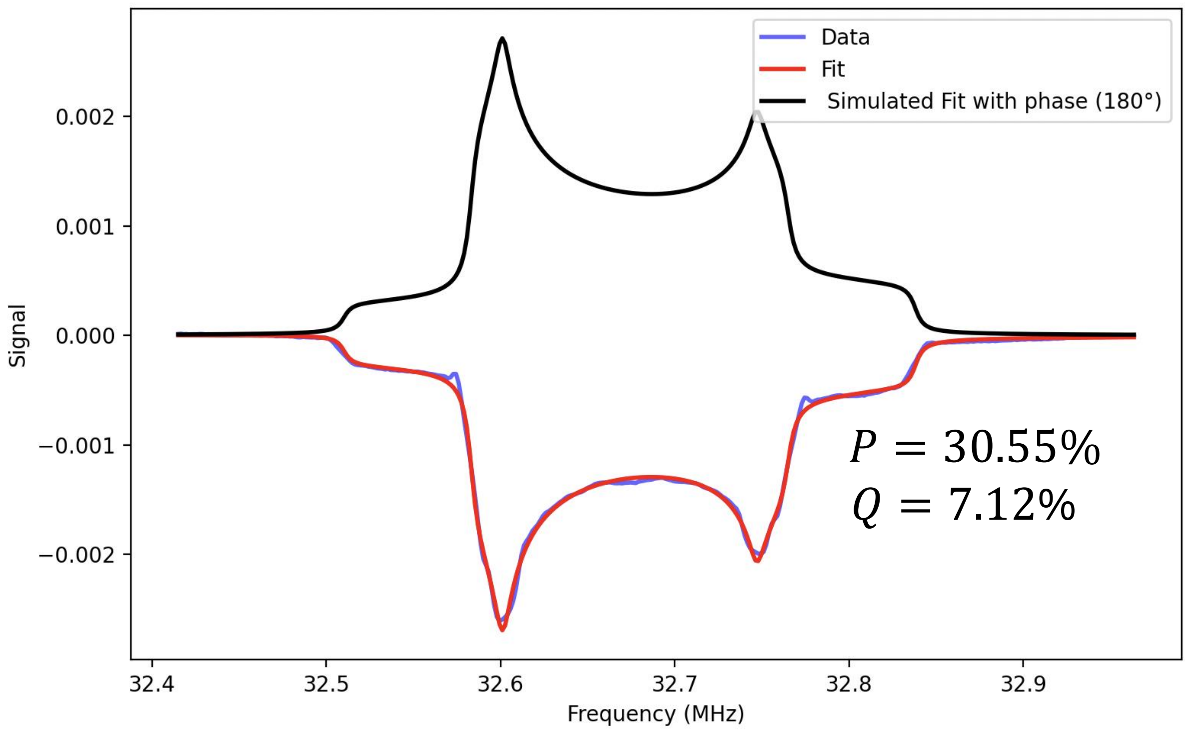
Mixed phase(simulation) continued

RGC 2022 data



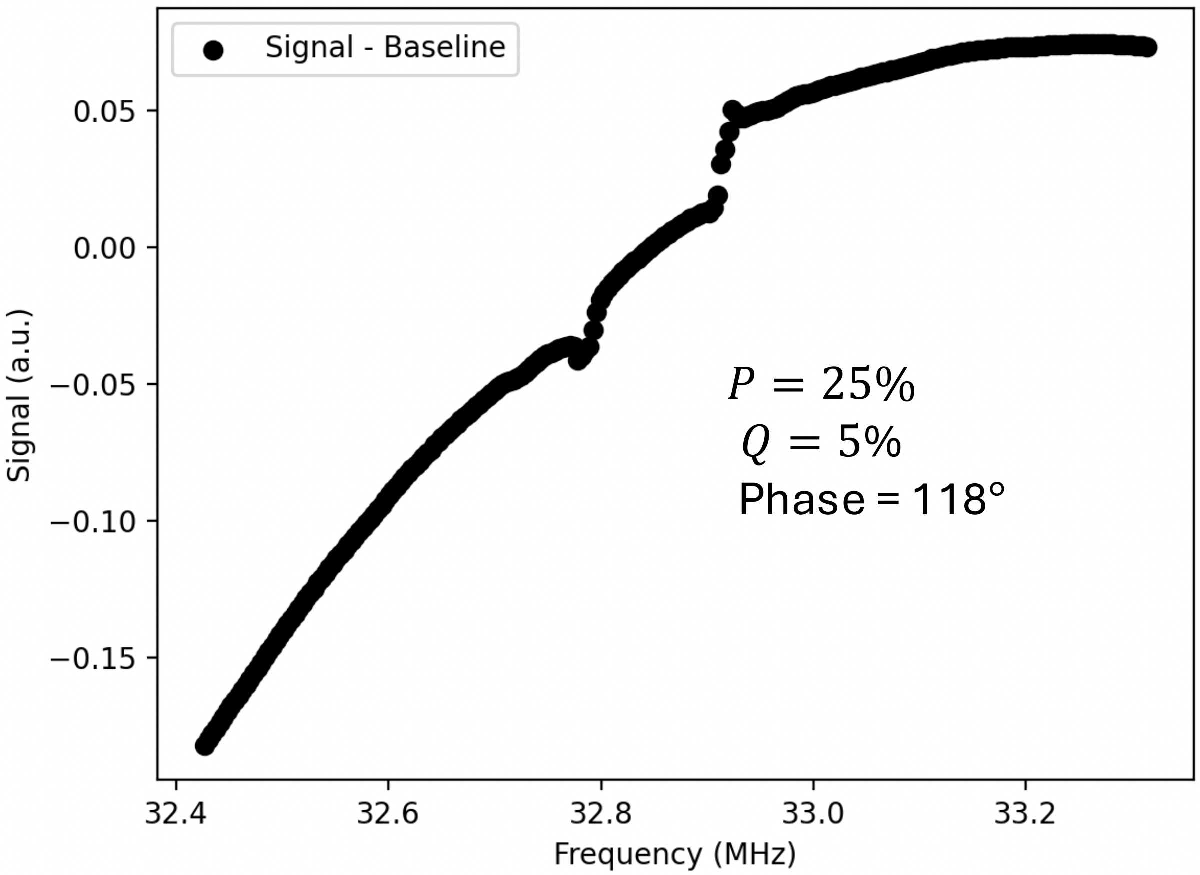
Data with Fit and simulated phase

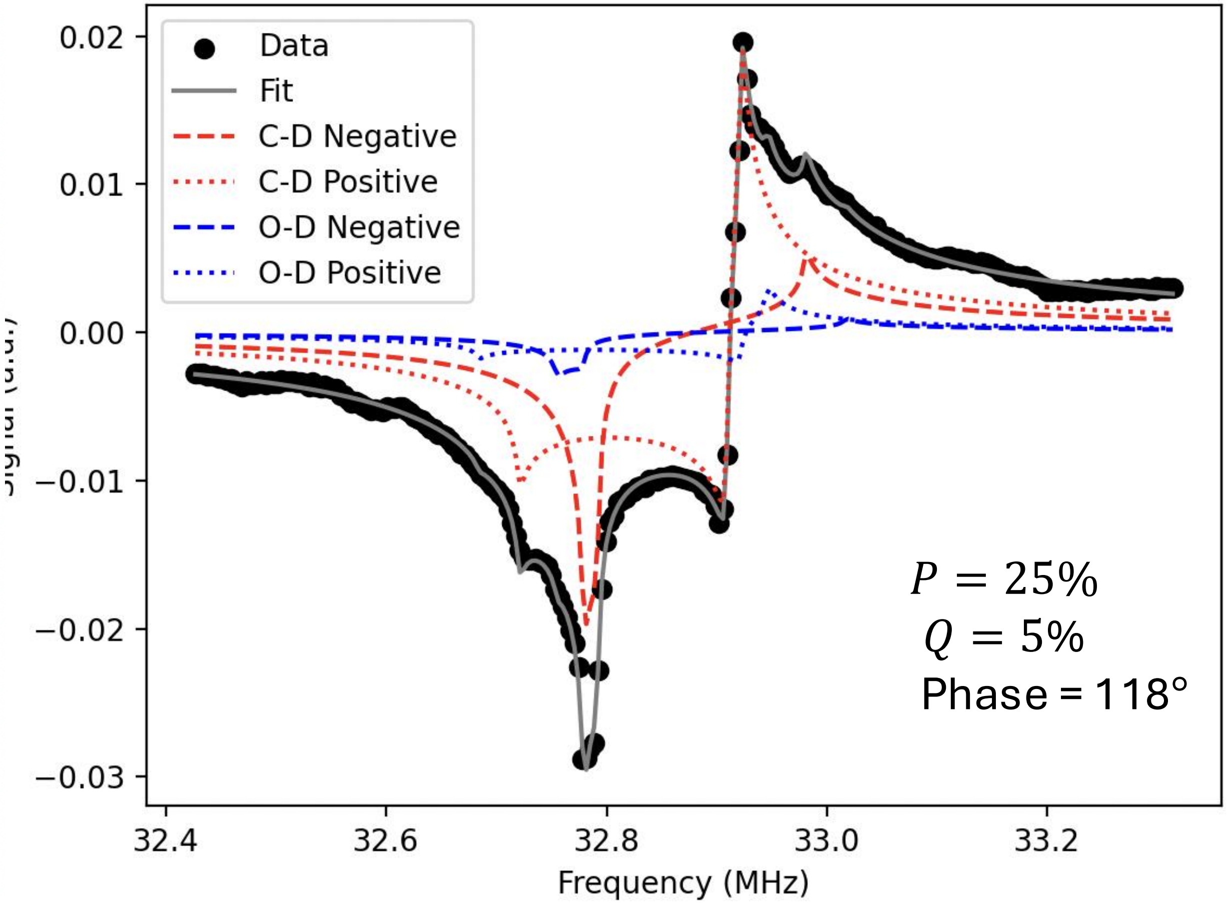


Data with Fit and simulated phase

Dulya et al., NIM A **398**, 109 (1997) https://github.com/jdmax/jlab_pynmr McClellan, Eur. Phys. J. A 61, 176 (2025)

Complex Fit





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https://github.com/jdmax/jlab_pynmr

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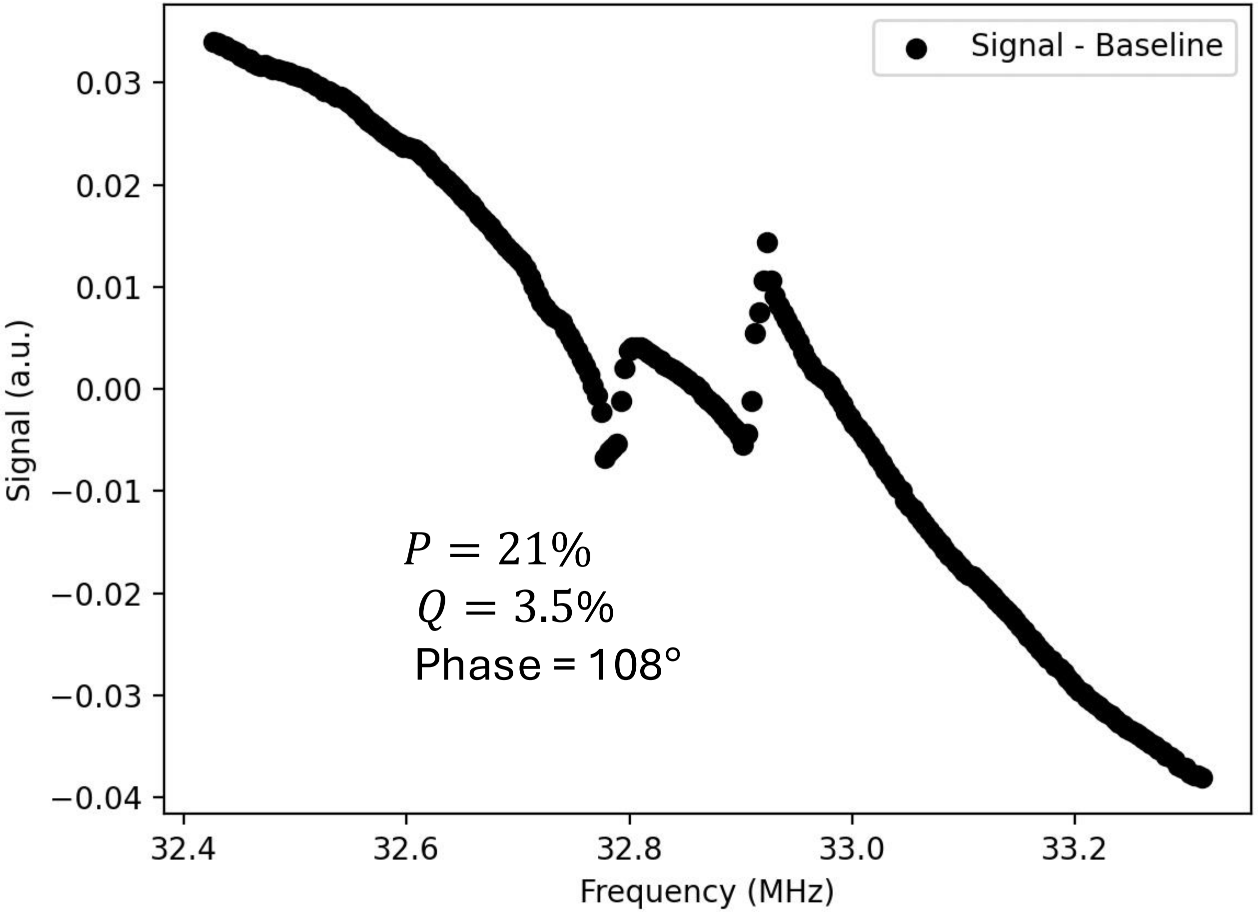
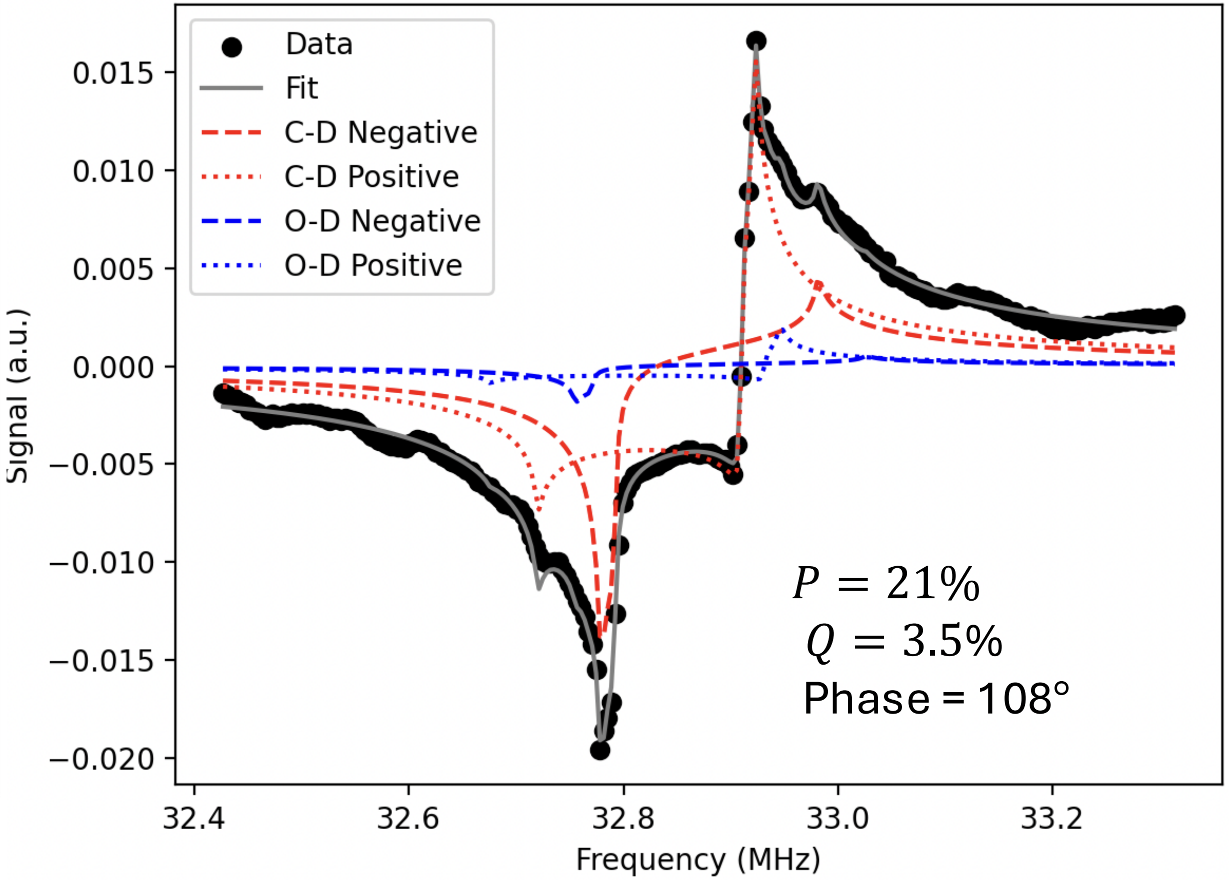
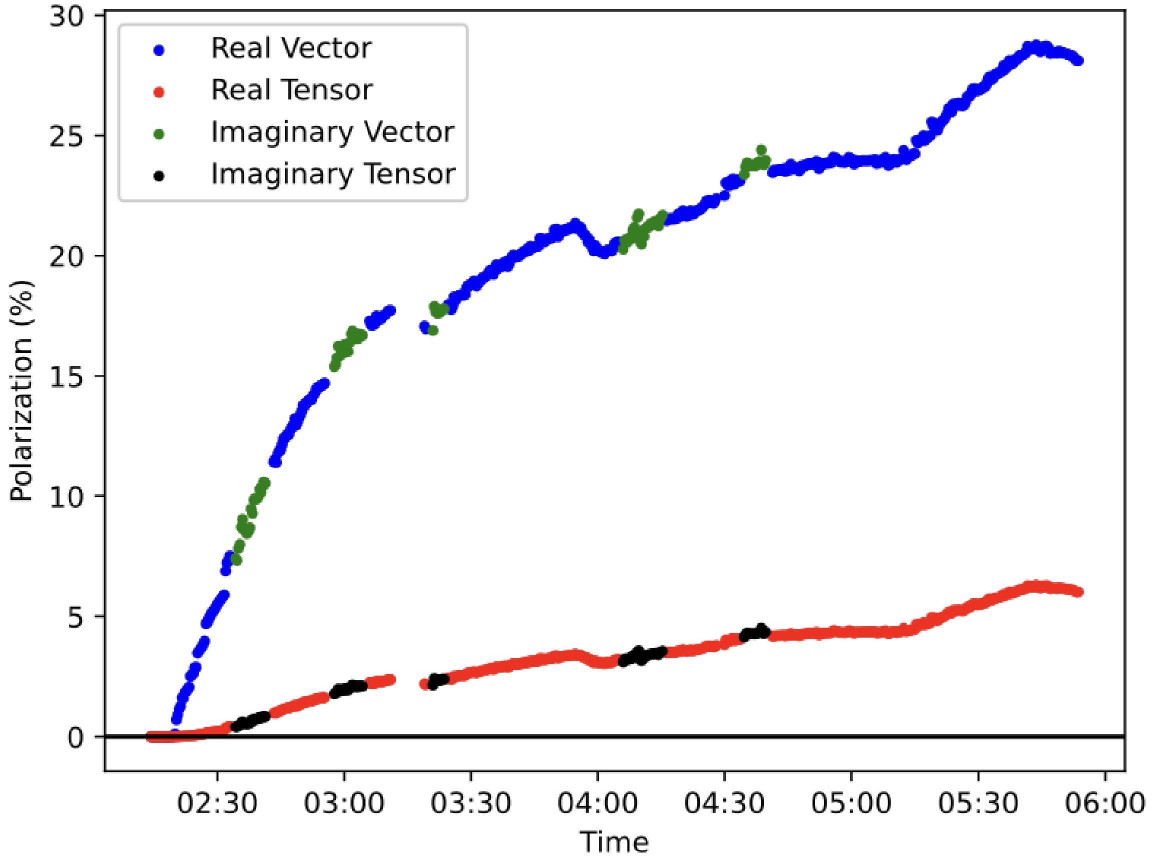
Complex Fit continued

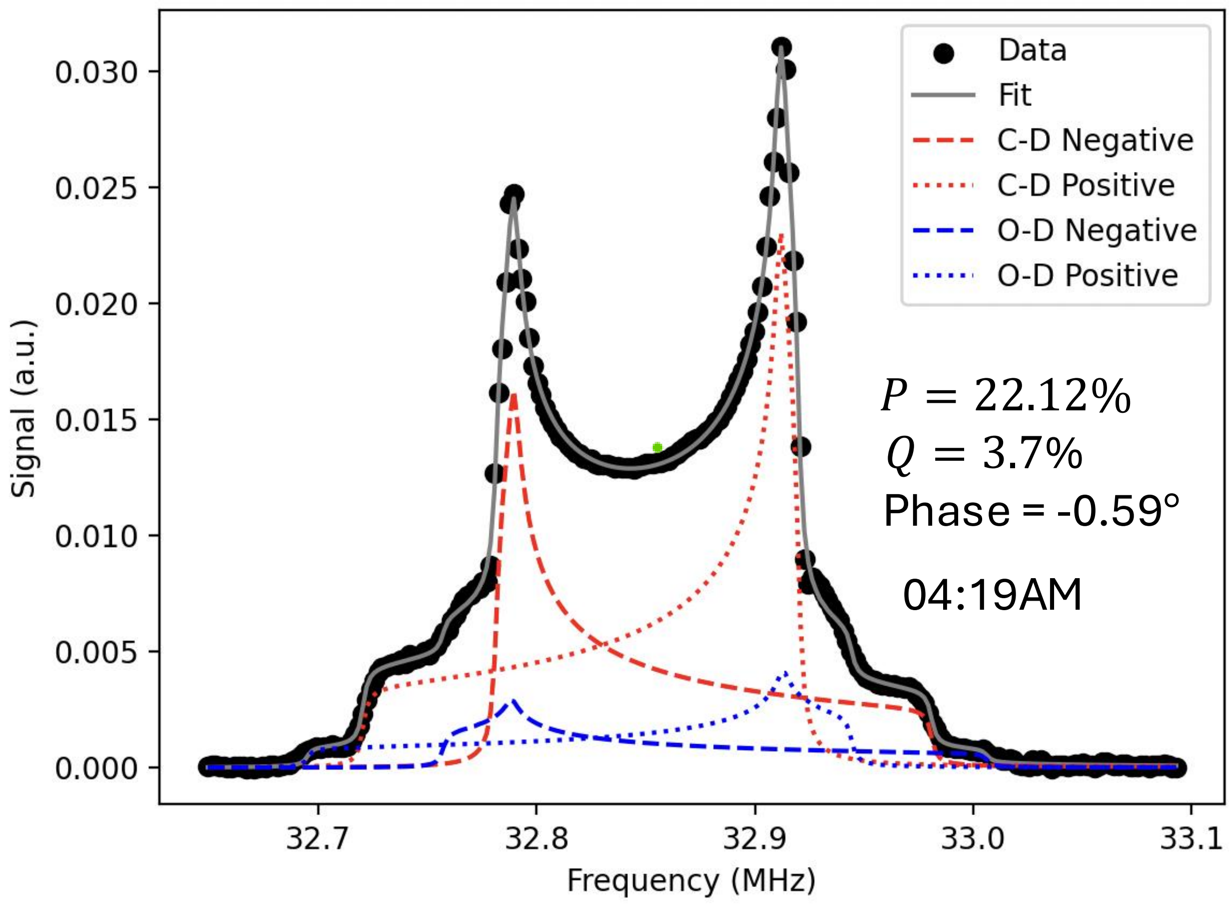




Dulya et al., NIM A **398**, 109 (1997) https://github.com/jdmax/jlab_pynmr McClellan, Eur. Phys. J. A 61, 176 (2025)

Complex Fit continued





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https://github.com/jdmax/jlab_pynmr

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Conclusion

- ✓ Complex signal implementation will follow data more closely than with out it.
- ✓ It has more fitting parameters but faster calculation
- ✓ This will help us reduce the systematic uncertainties in the future experiments like b1 and Azz, Run Group C.
- ✓ This can be found in github.

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https://github.com/jdmax/jlab_pynmr

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Backup Slides

$$Y = \sqrt{3 - \eta\cos(2\phi)}$$

$$f_\varepsilon(R, A, \eta, \phi) = \frac{1}{2\pi\varrho}\left\{2\cos(\alpha/2)\left[\arctan\left(\frac{Y^2-\varrho^2}{2Y\varrho\sin(\alpha/2)}\right)+\frac{\pi}{2}\right] + \sin(\alpha/2)\ln\left(\frac{Y^2+\varrho^2+2Y\varrho\cos(\alpha/2)}{Y^2+\varrho^2-2Y\varrho\cos(\alpha/2)}\right)\right\},$$

where $\varrho^2 = \sqrt{A^2 + [1 - \varepsilon R - \eta\cos(2\phi)]^2}$, $\cos(\alpha) = [1 - \varepsilon R - \eta\cos(2\phi)]/\varrho^2$.

$$D(\omega) = 1 + \tfrac{1}{2}\xi(1 + R), \qquad (28)$$

where ξ is the false asymmetry parameter. The equation is written in this manner so that ξ is directly the difference in gain between the two peaks of the signal. Now, the false asymmetry correction to χ'' is put

M. McClellan, Ph.D. thesis, Uninversity of New Hampshire, 2026

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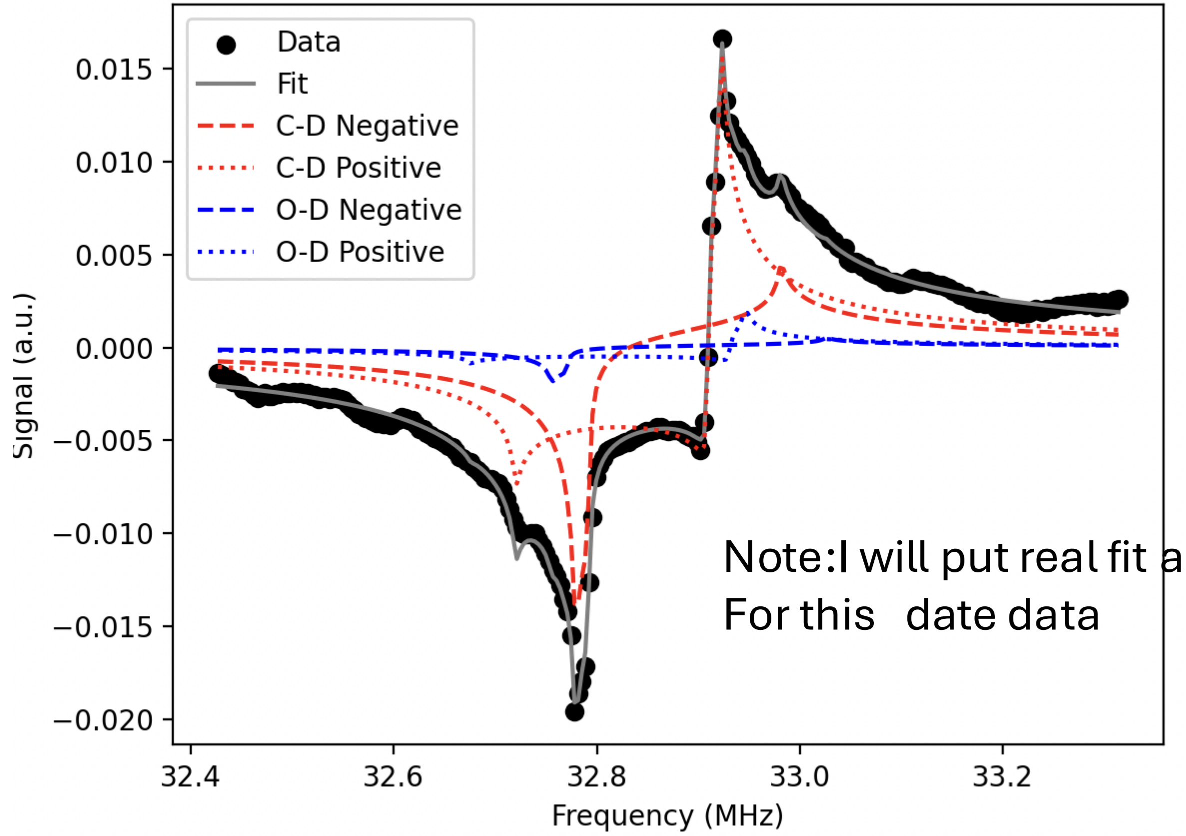
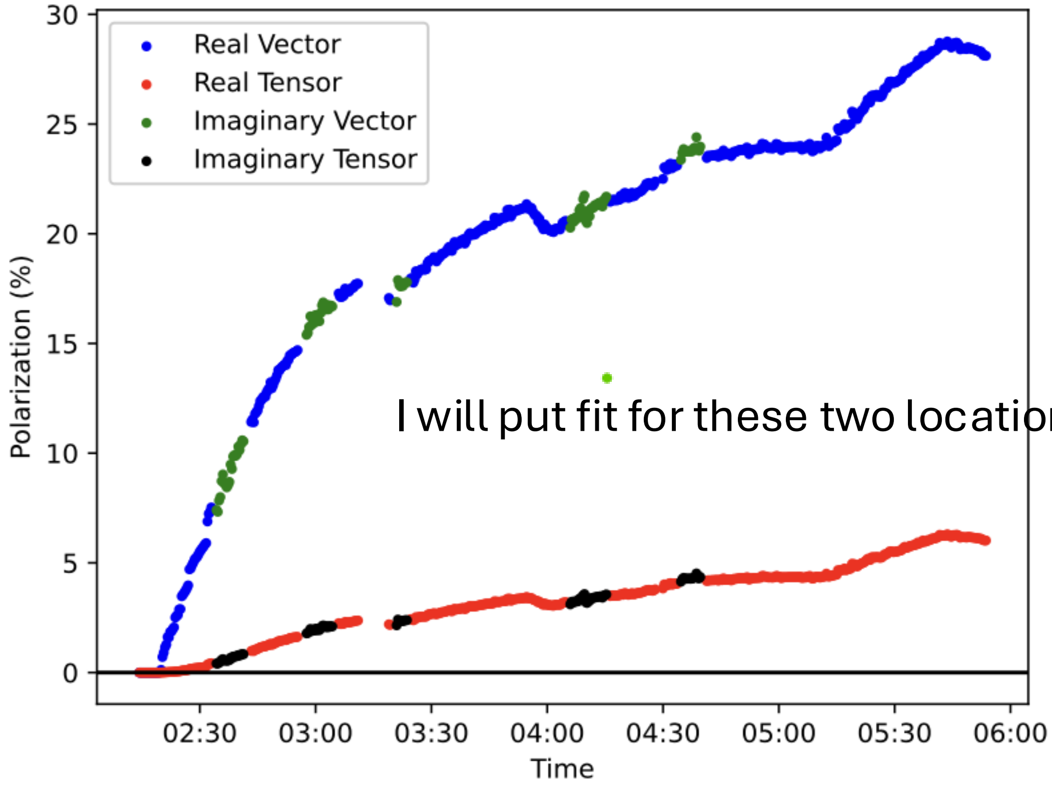
Complex Fit continued

<u>Backup Slides</u>



Note:I will put real fit also
For this date data



I will put fit for these two location

M. McClellan, Ph.D. thesis, University of New Hampshire, 2026

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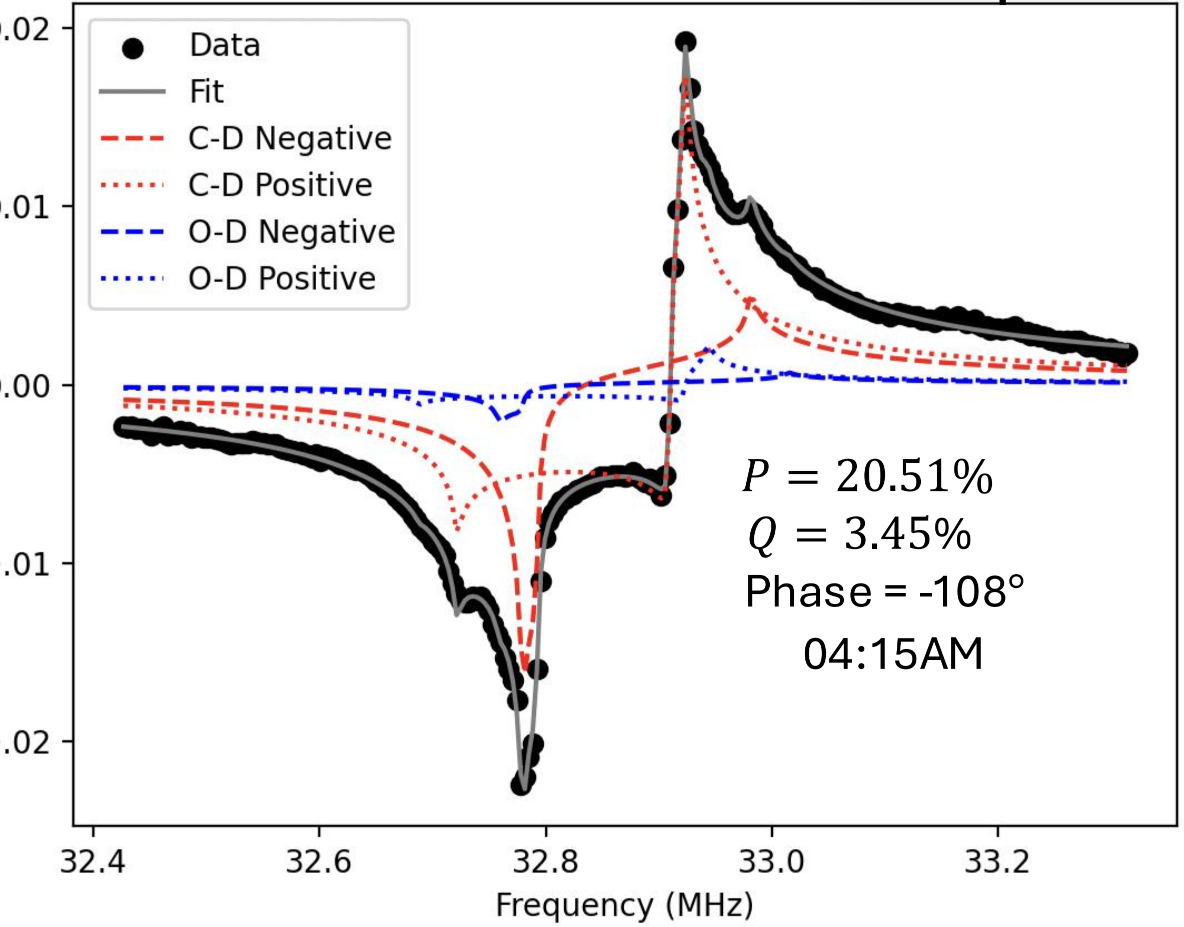
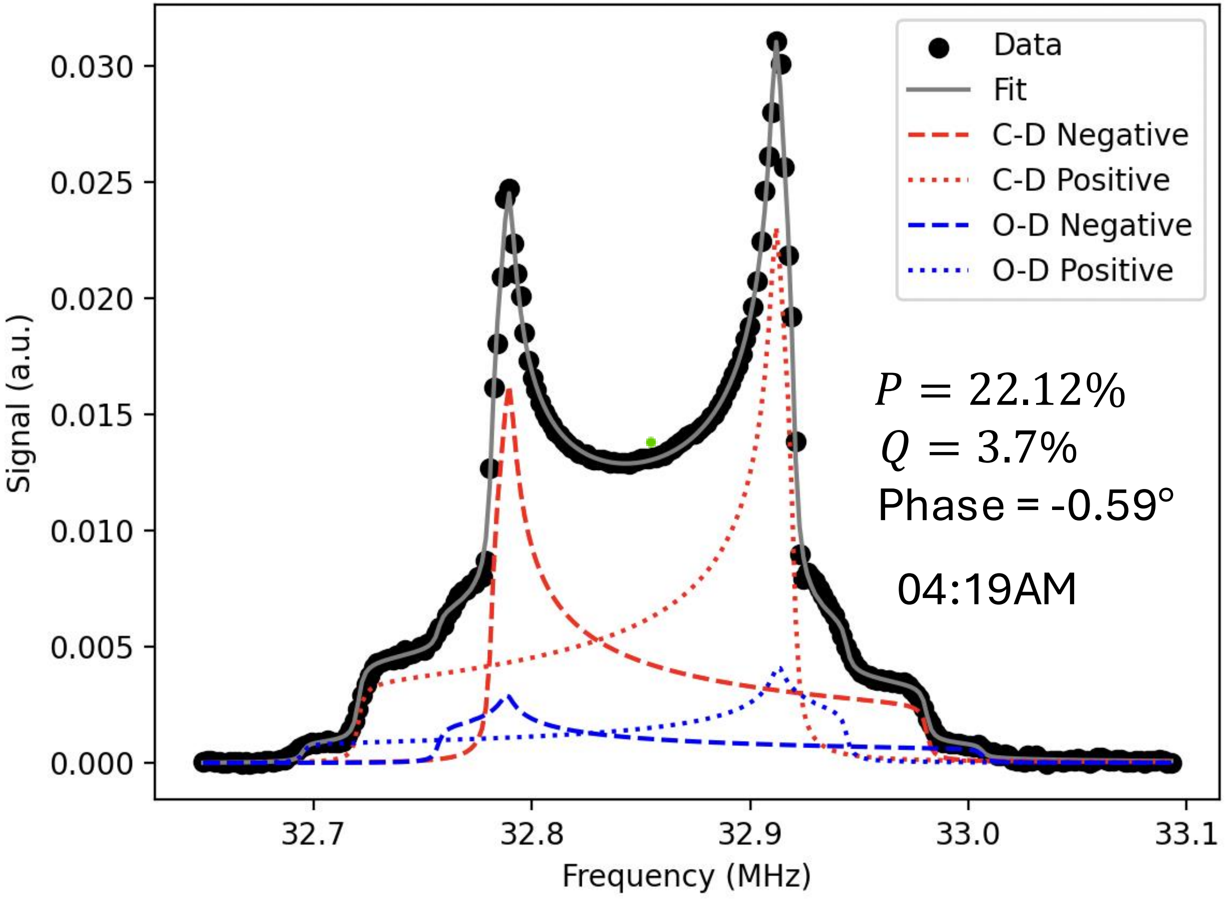
Complex Fit continued

Backup Slides





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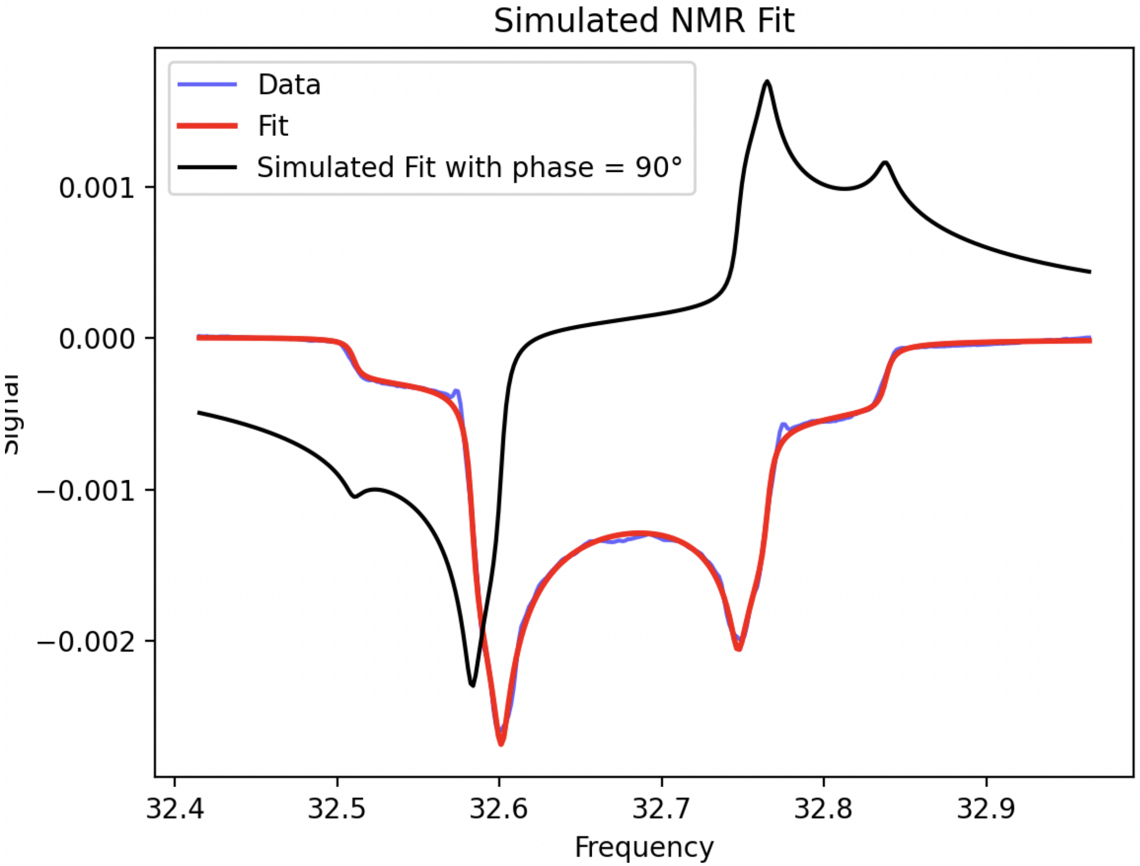
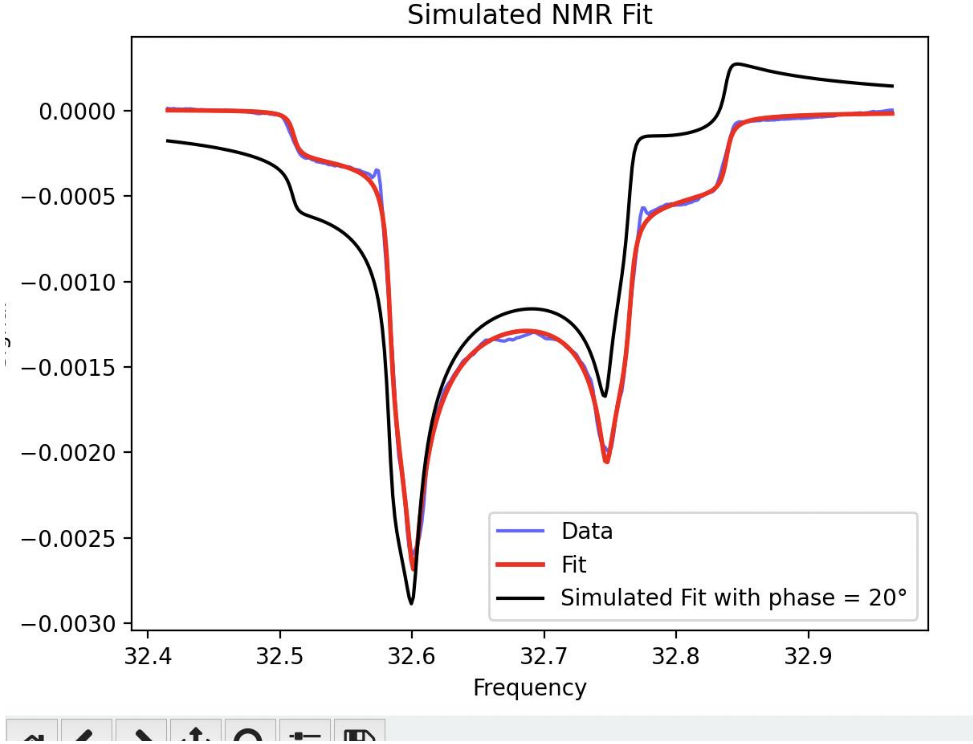
There are two types of the plots in the simulation I am confused and which one is correct??
From slide number 13 to 17





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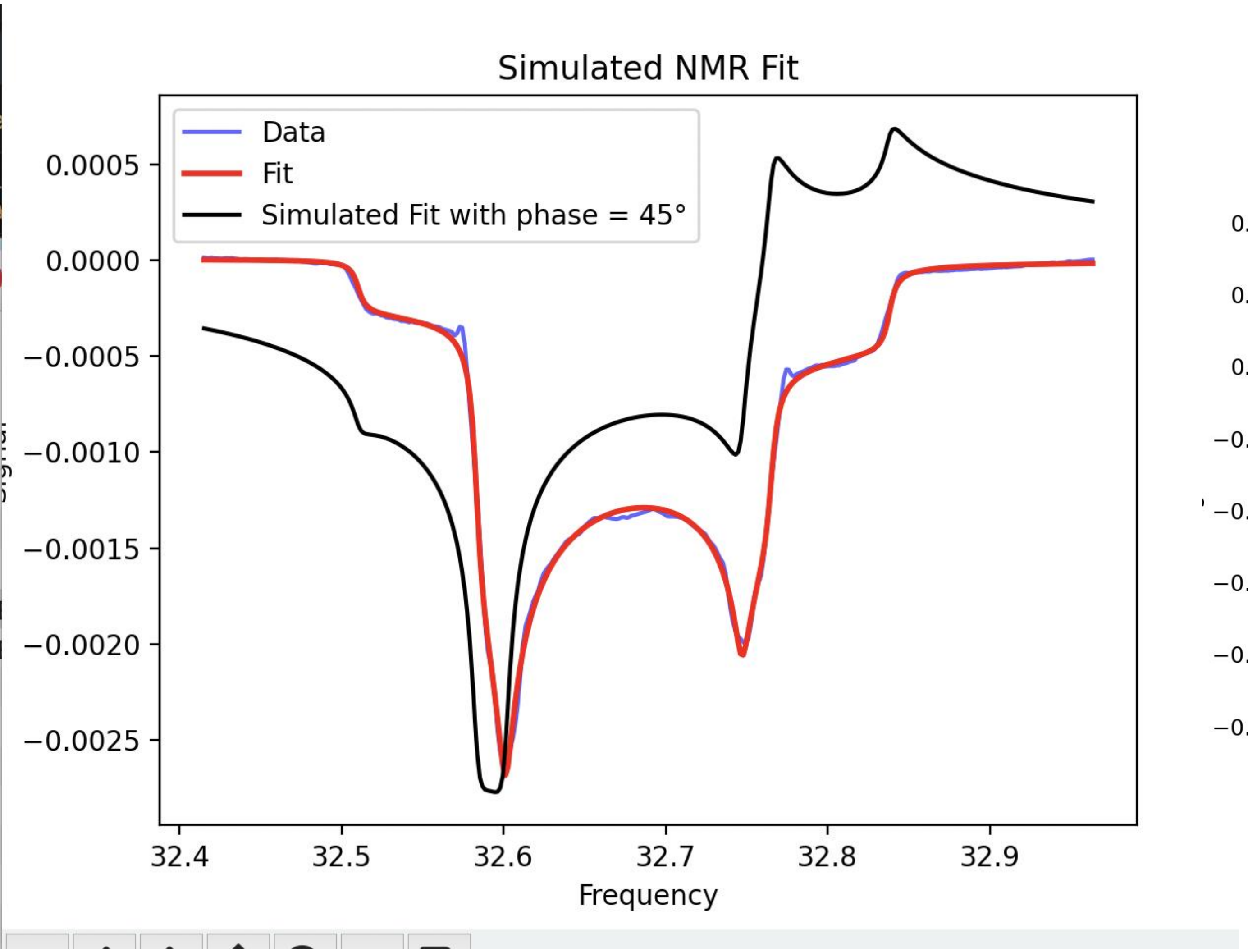

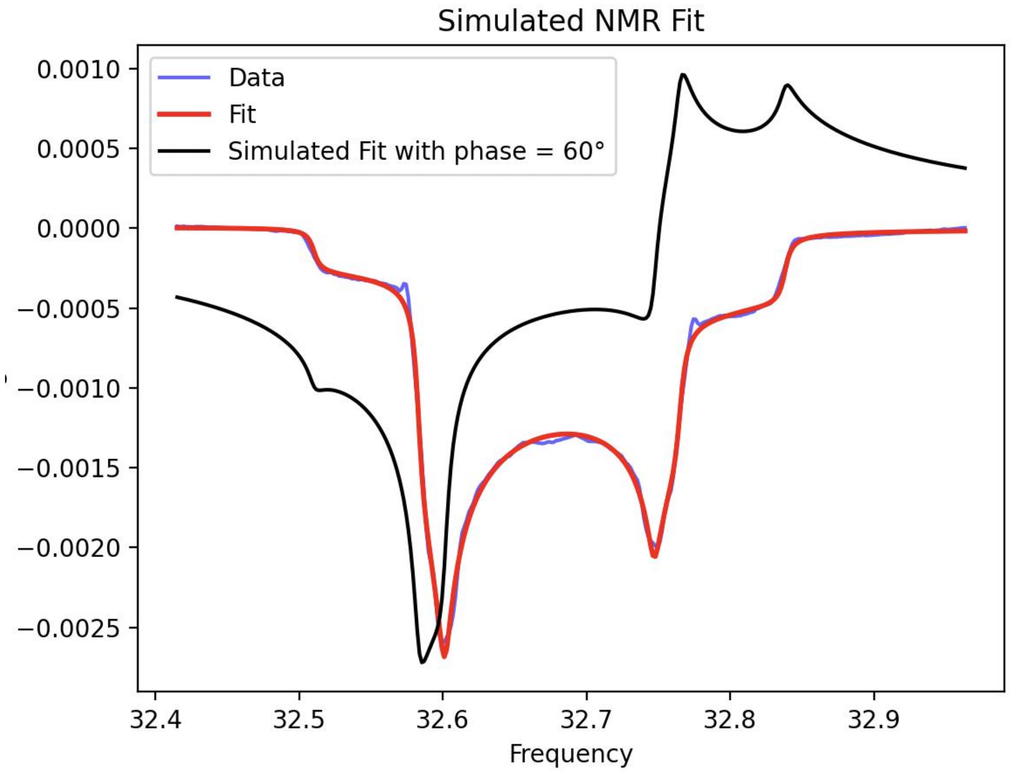

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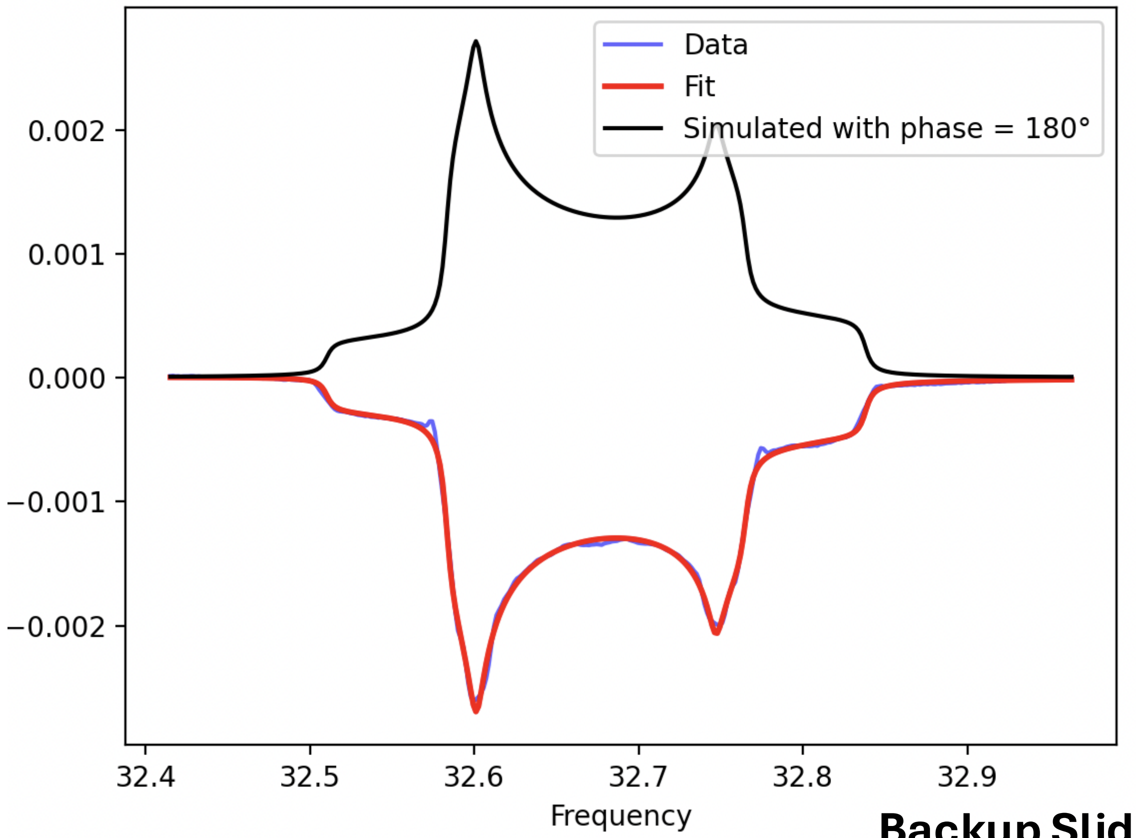

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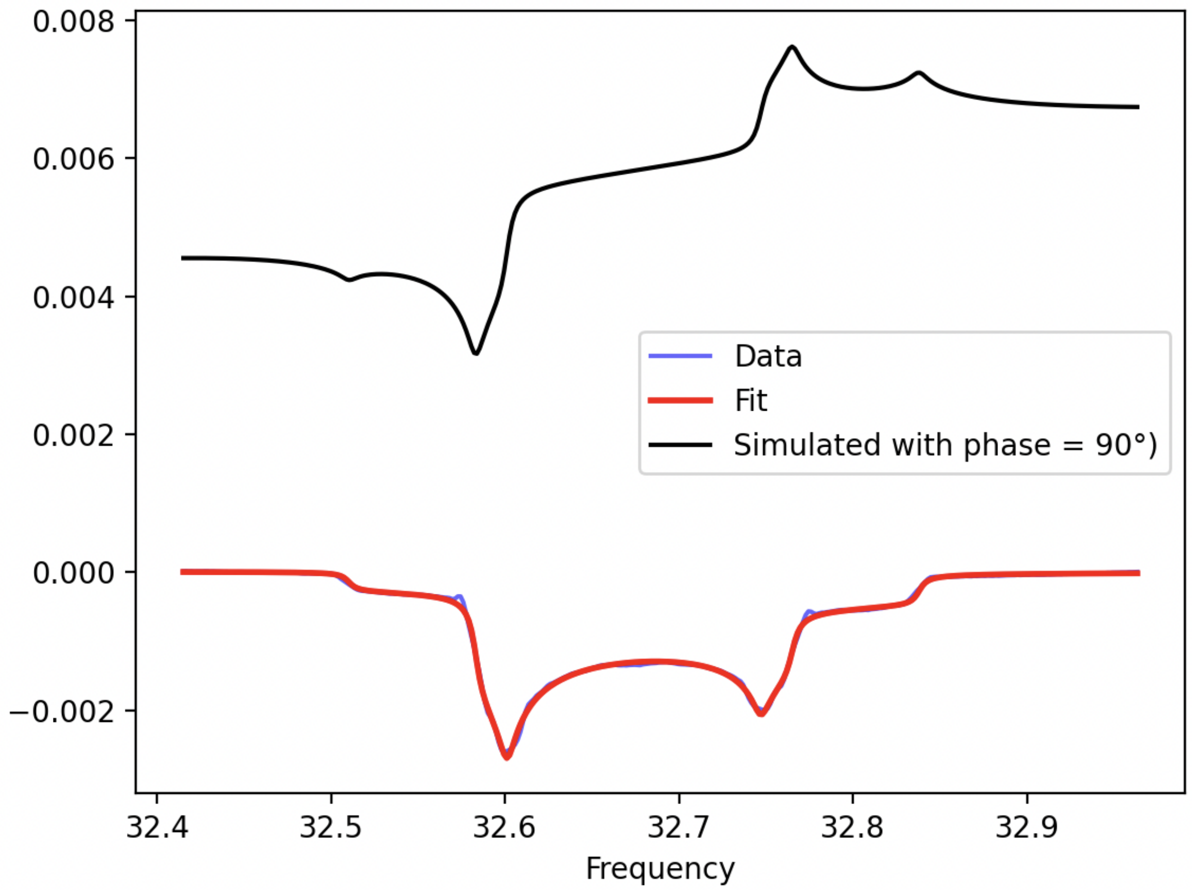

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