Advances In Solid-Target Tensor Polarization

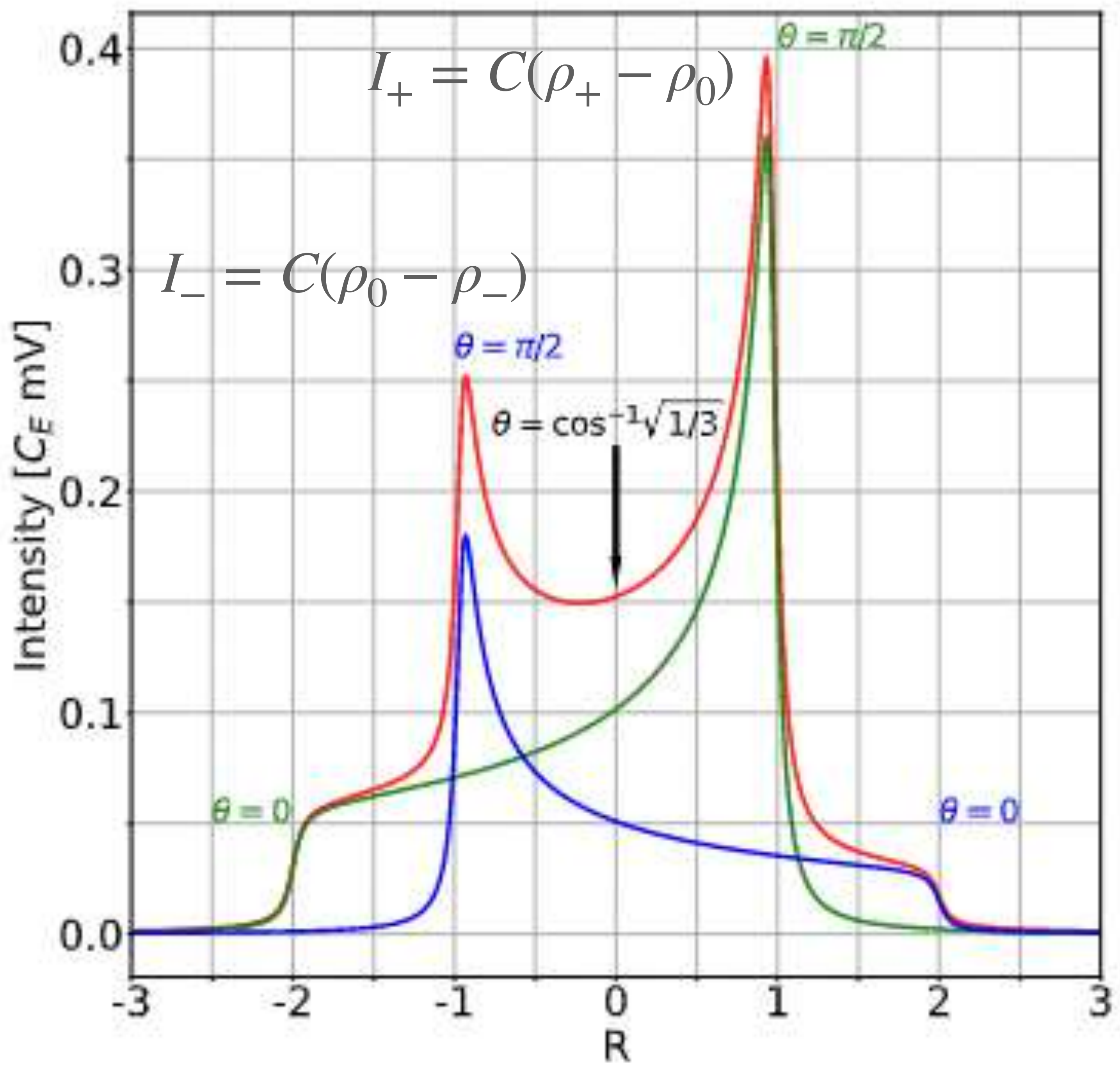
Conditional Review

D Keller

Contents

Deuteron Polarization

CW-NMR in Polycrystalline Samples



$$I_+ = C(\rho_+ - \rho_0)$$

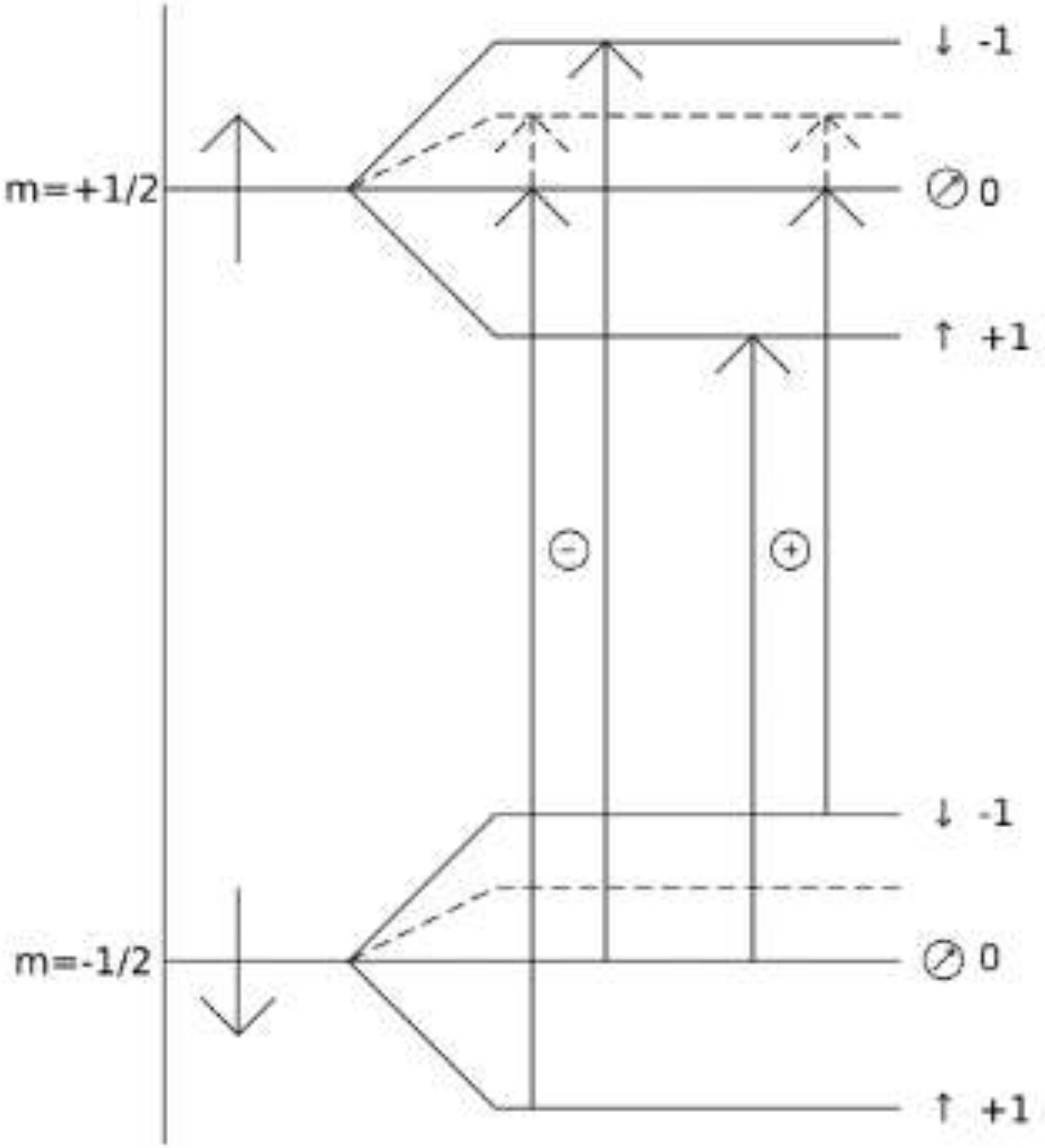
$$I_- = C(\rho_0 - \rho_-)$$

$$R = \frac{\omega - \omega_d}{3\omega_q}$$

$$P = \frac{\rho_+ - \rho_-}{\rho_+ + \rho_0 - \rho_-}$$

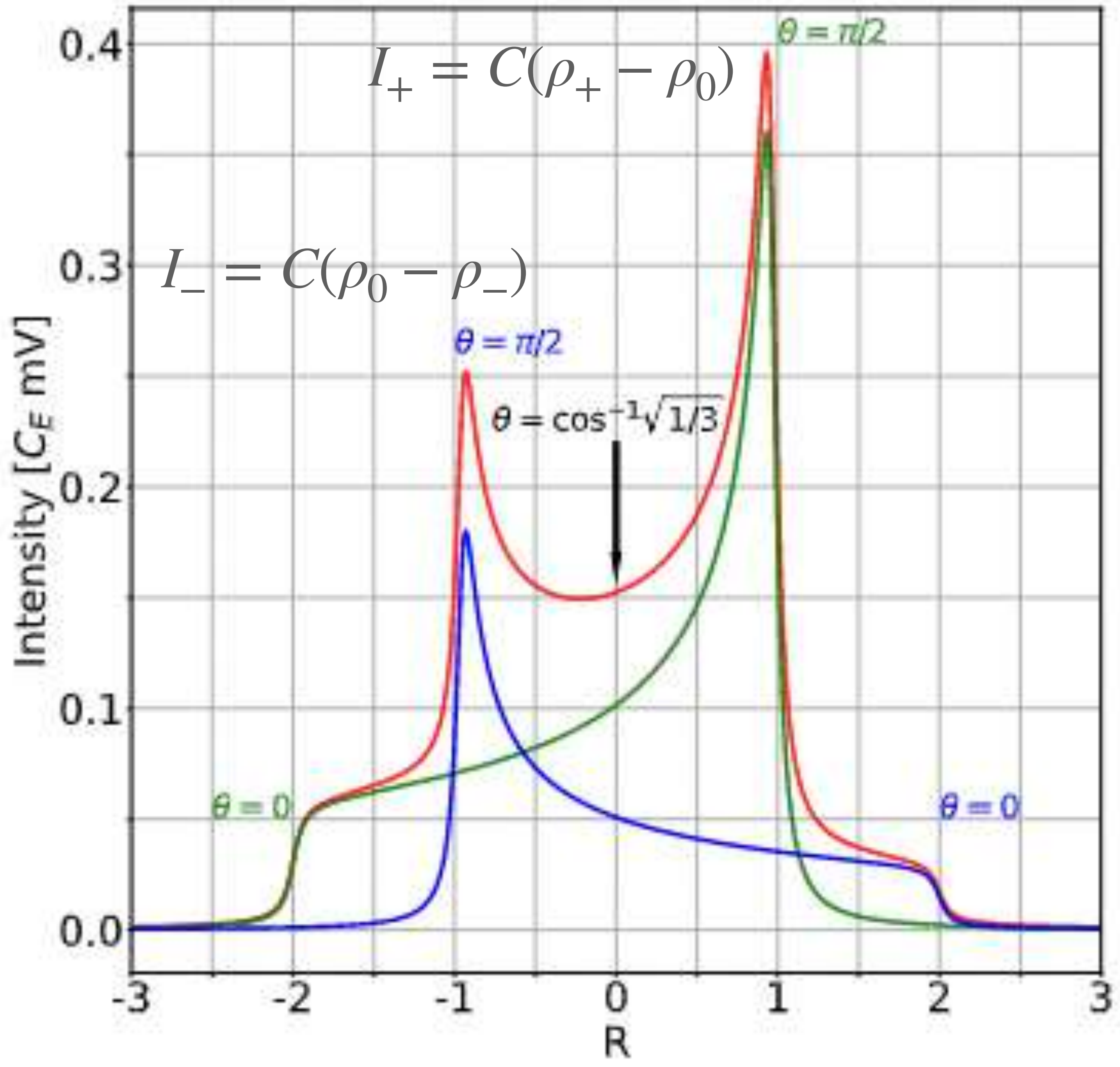
$$Q = \frac{\rho_+ + \rho_- - 2\rho_0}{\rho_+ + \rho_0 - \rho_-}$$

$$\mathscr{F} = \frac{1}{2\pi\mathscr{X}}\left[2\cos(\alpha/2)\left(\arctan\left(\frac{\mathscr{Y}^2 - \mathscr{X}^2}{2\mathscr{Y}\mathscr{X}\sin(\alpha/2)}\right) + \frac{\pi}{2}\right)\right.$$
$$\left. + \sin(\alpha/2)\ln\left(\frac{\mathscr{Y}^2 + \mathscr{X}^2 + 2\mathscr{Y}\mathscr{X}\cos(\alpha/2)}{\mathscr{Y}^2 + \mathscr{X}^2 - 2\mathscr{Y}\mathscr{X}\cos(\alpha/2)}\right)\right],$$



Deuteron Polarization

CW-NMR in Polycrystalline Samples



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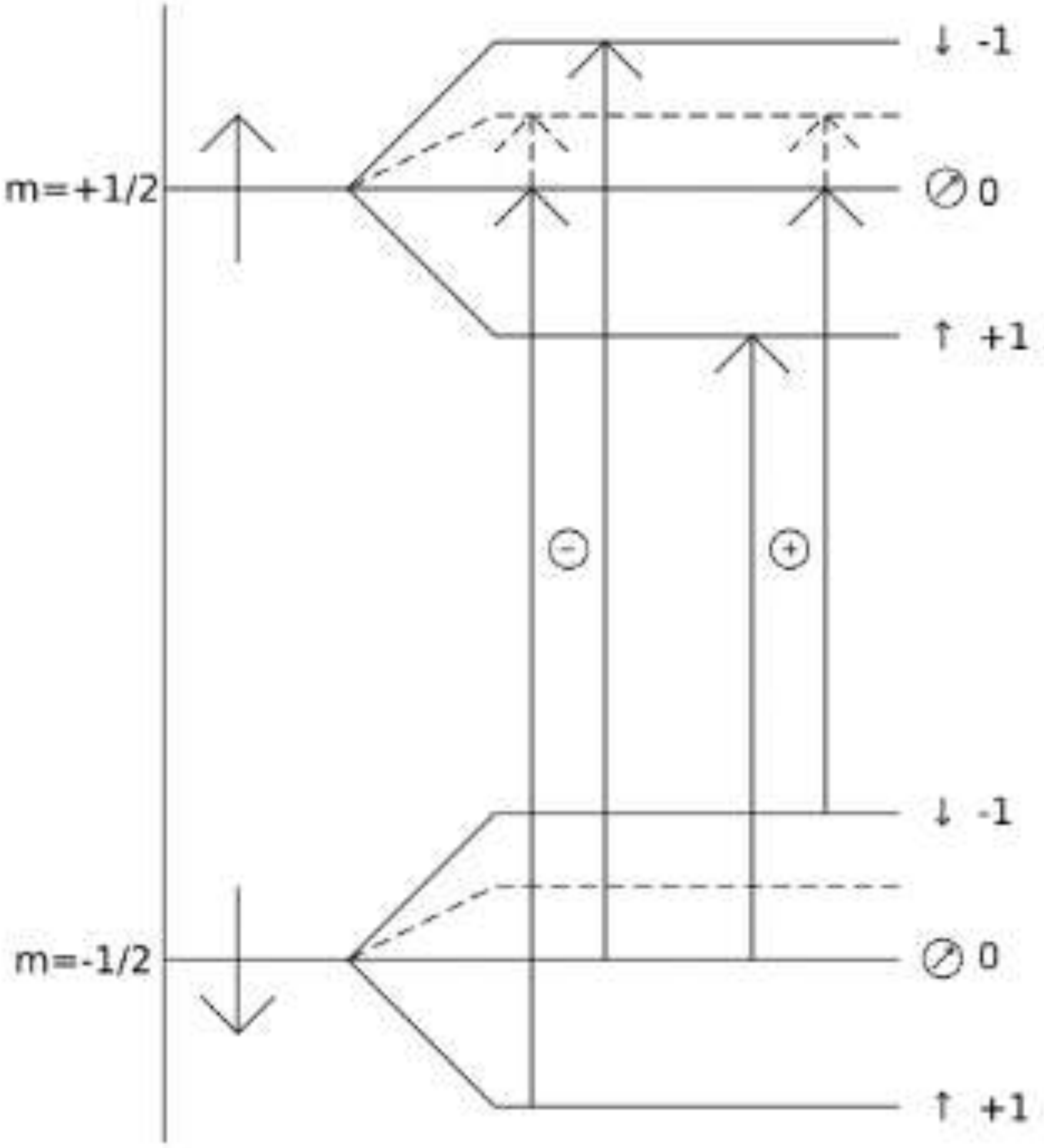
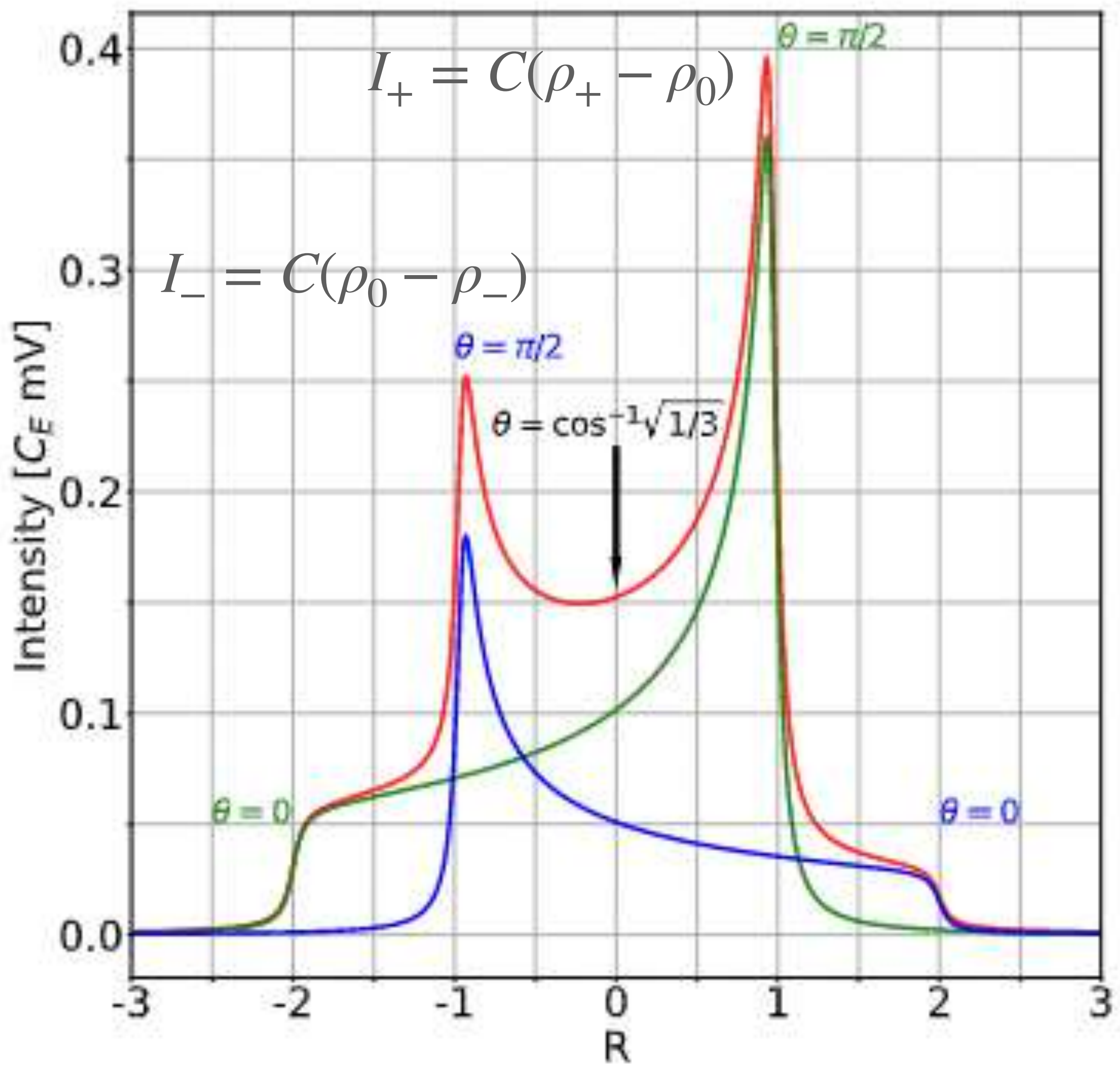
$$R = \frac{\omega - \omega_d}{3\omega_q}$$

$$P = C(I_+ + I_-) = C([\rho_+ - \rho_0] + [\rho_0 - \rho_-])$$
$$Q = C(I_+ - I_-) = C([\rho_+ - \rho_0] - [\rho_0 - \rho_-])$$



Deuteron Polarization

CW-NMR in Polycrystalline Samples



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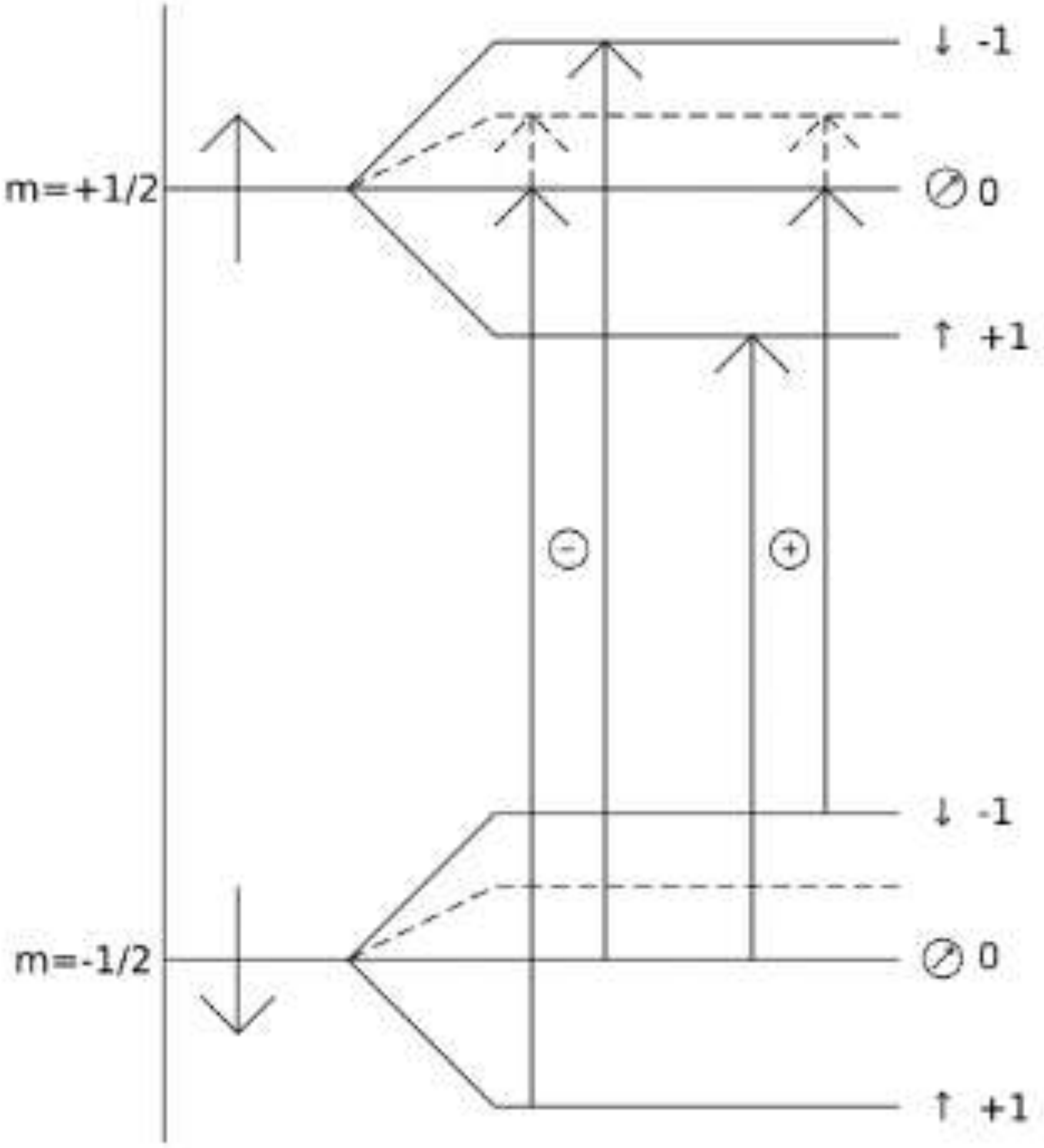
$$P = \frac{\rho_+ - \rho_-}{\rho_+ + \rho_0 - \rho_-}$$

$$Q = \frac{\rho_+ + \rho_- - 2\rho_0}{\rho_+ + \rho_0 - \rho_-}$$

$$R = \frac{\omega - \omega_d}{3\omega_q}$$

$$P_{zz} = 2 - \sqrt{4 - 3P^2}$$



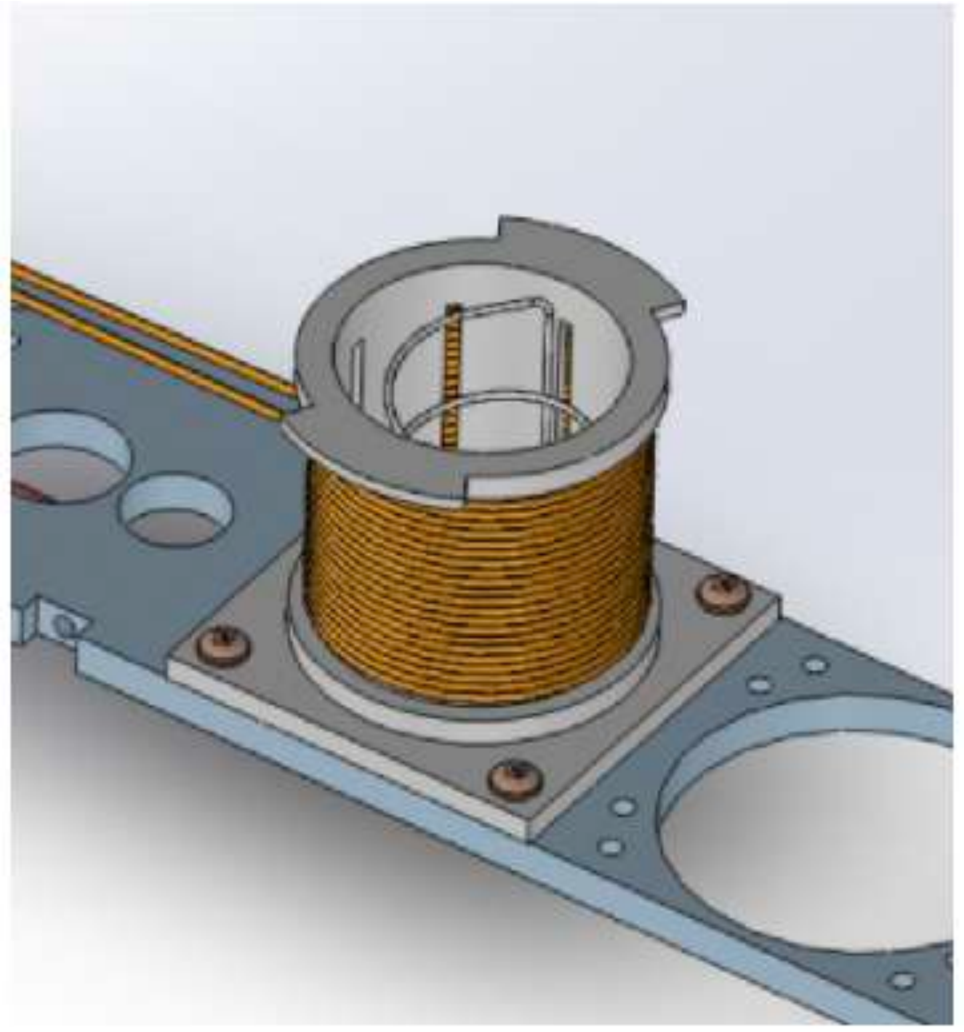
Charge-1

Technique to Enhance the Tensor Polarization

- We use Selective Semi-saturating RF to alter the energy level populations
    - RF close to Lamor frequency from a separate source than the DNP
    - Selective: Select the range in the frequency domain to RF
    - Semi-saturating: Monitor and respond using RF power control and timing
- Instrumentation is specialized to generate RF
    - Separate coil to apply SS-RF
    - Q-meter with RF switch
    - RF amplification with fine control and capacity to modulate rapidly over domain

Application of RF

In Selective Semi-saturation



$$P = C(I_+ + I_-)$$

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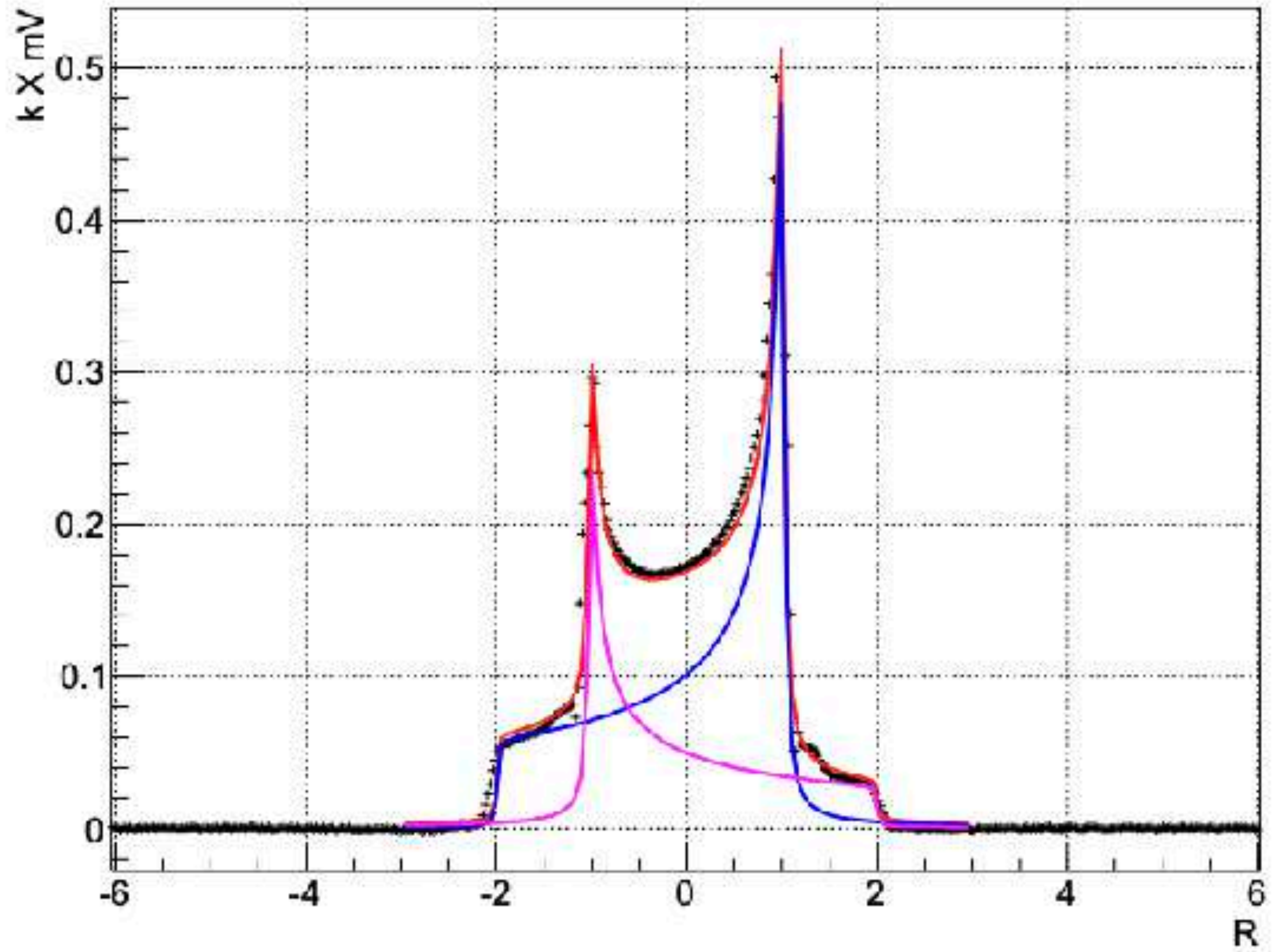

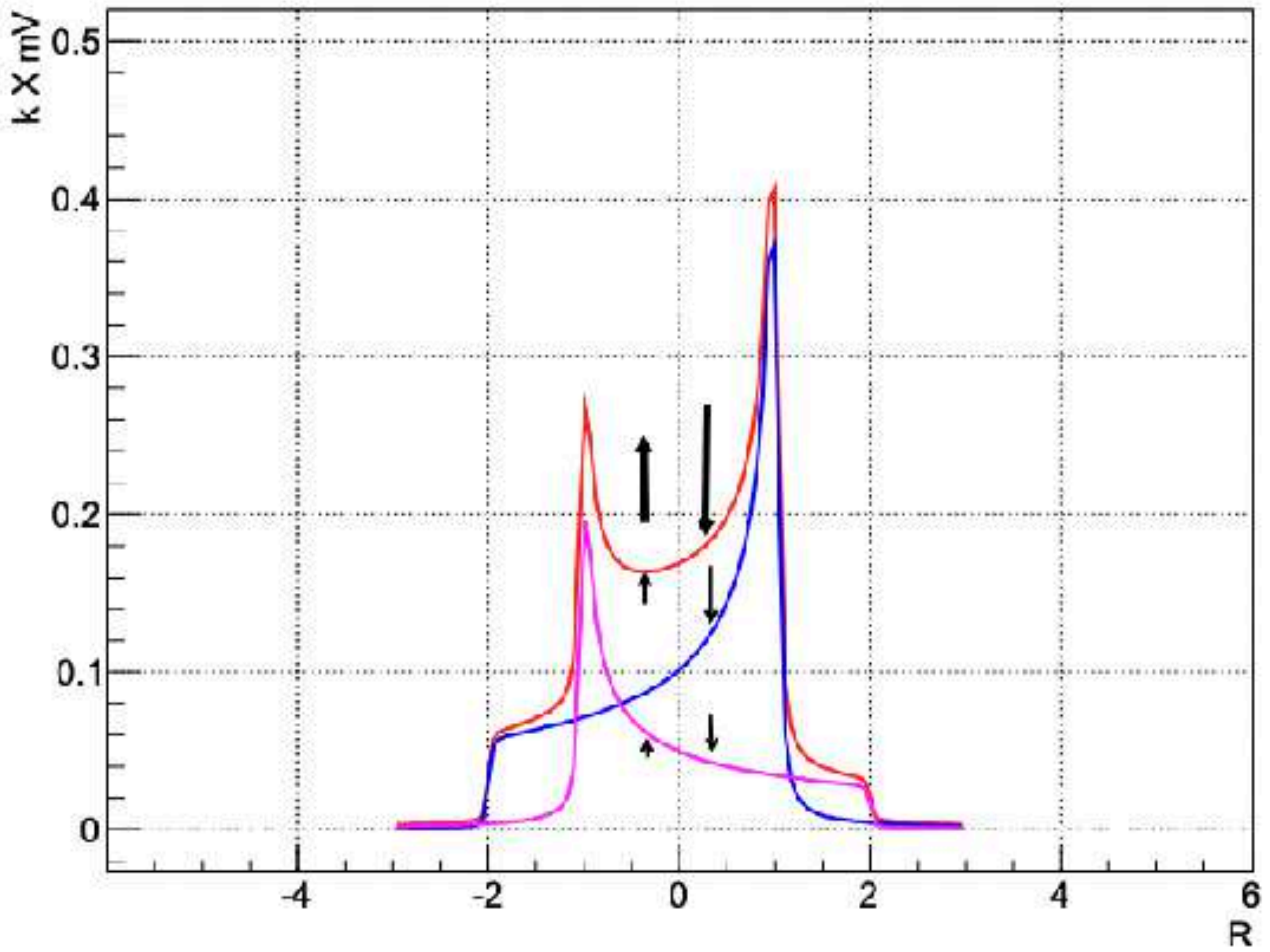

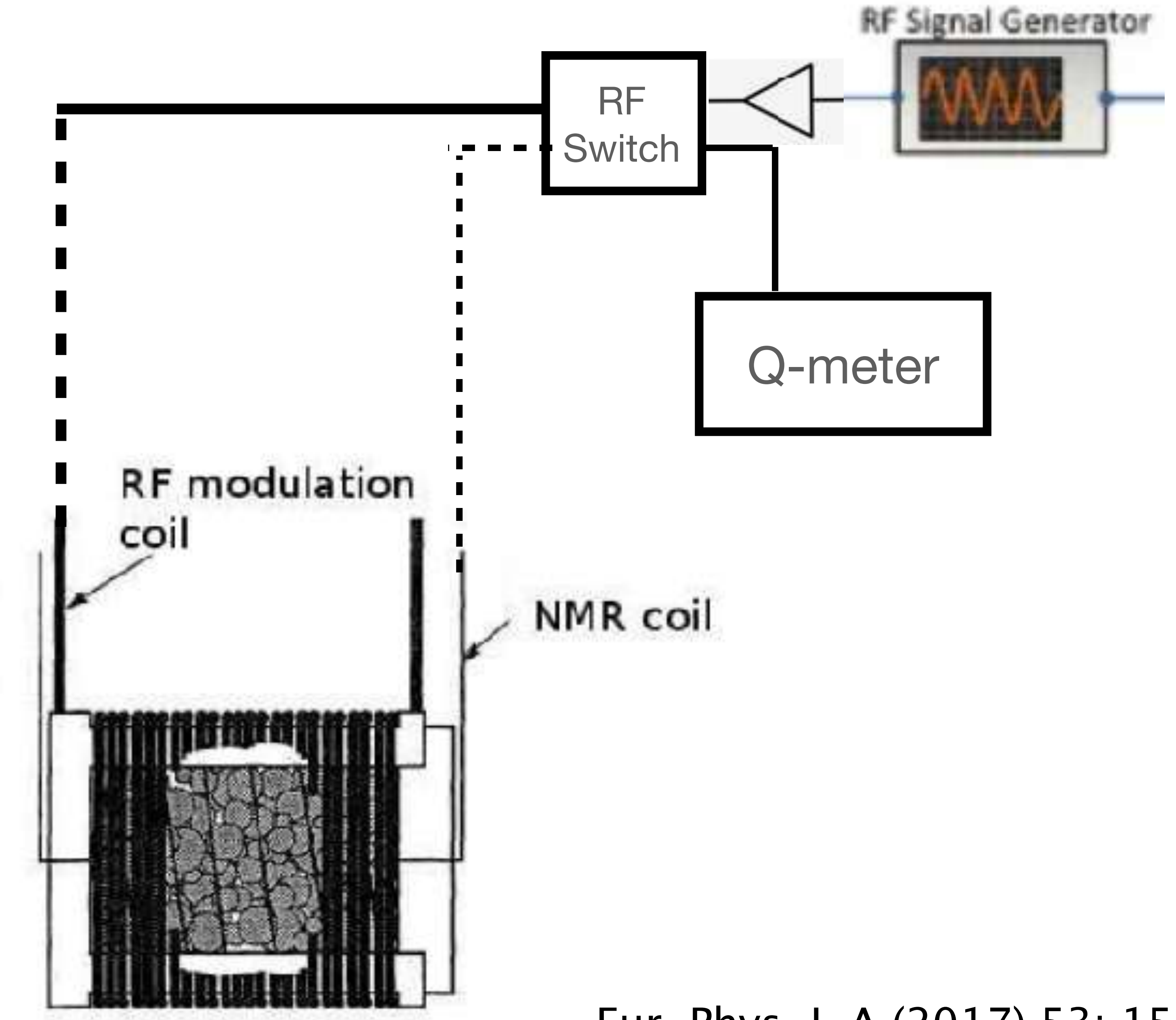

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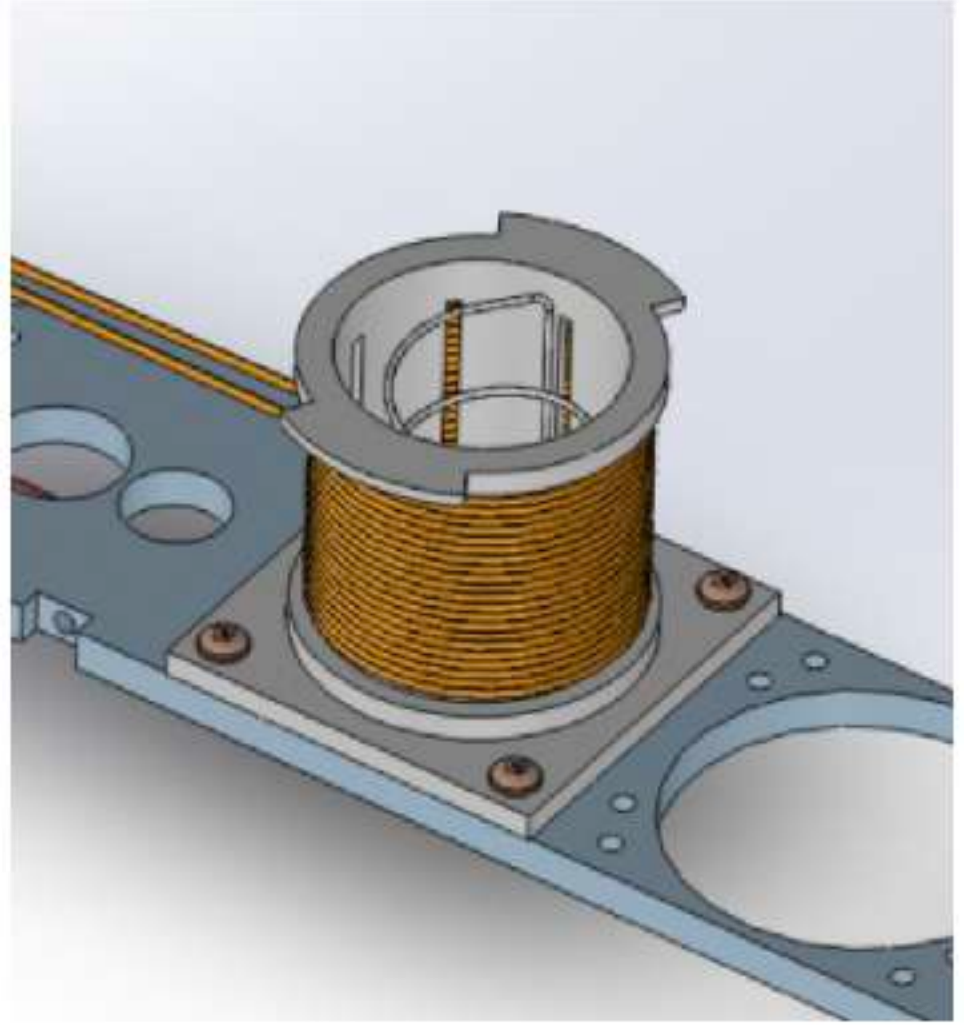
Application of RF

In Selective Semi-saturation



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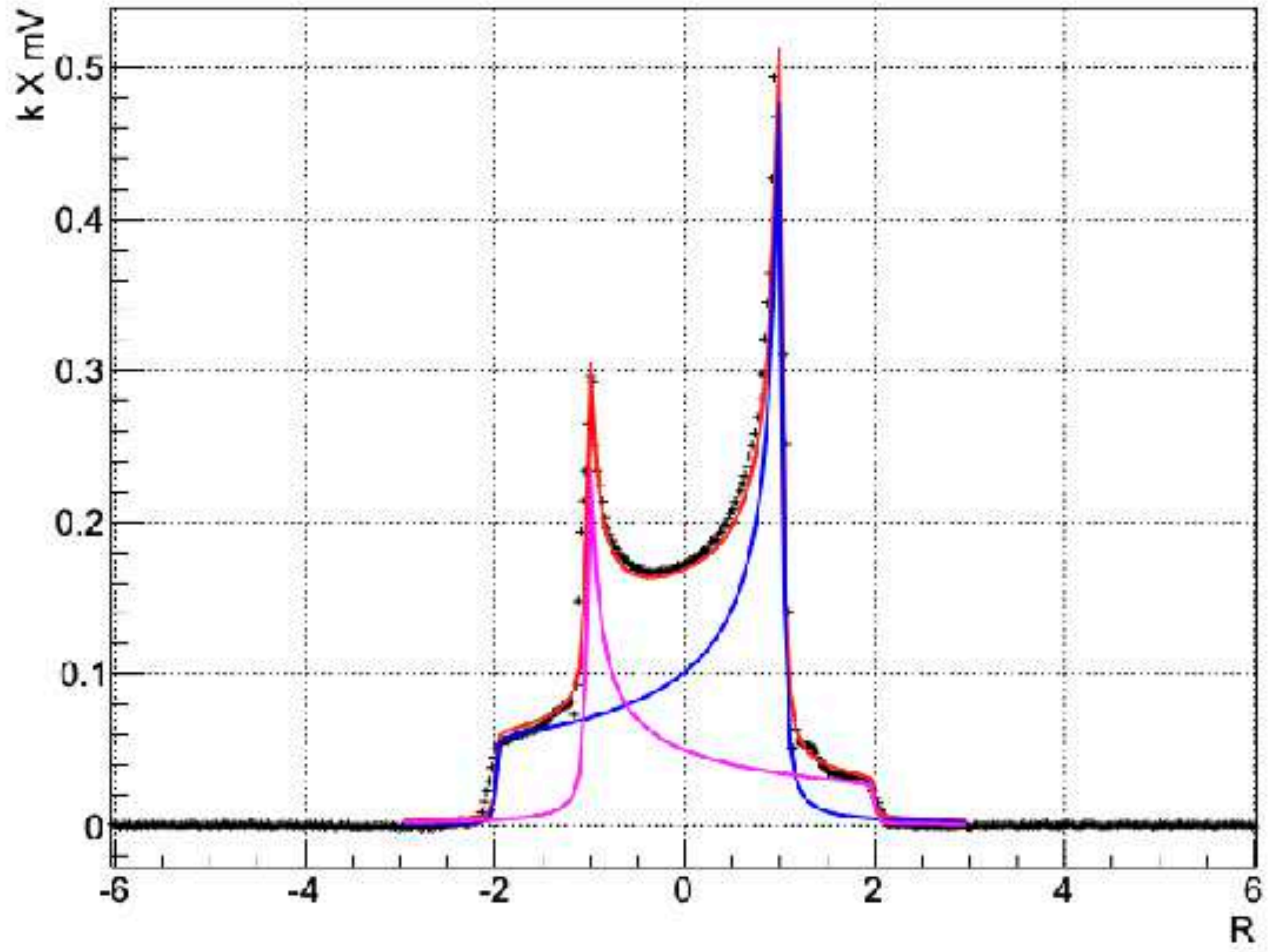

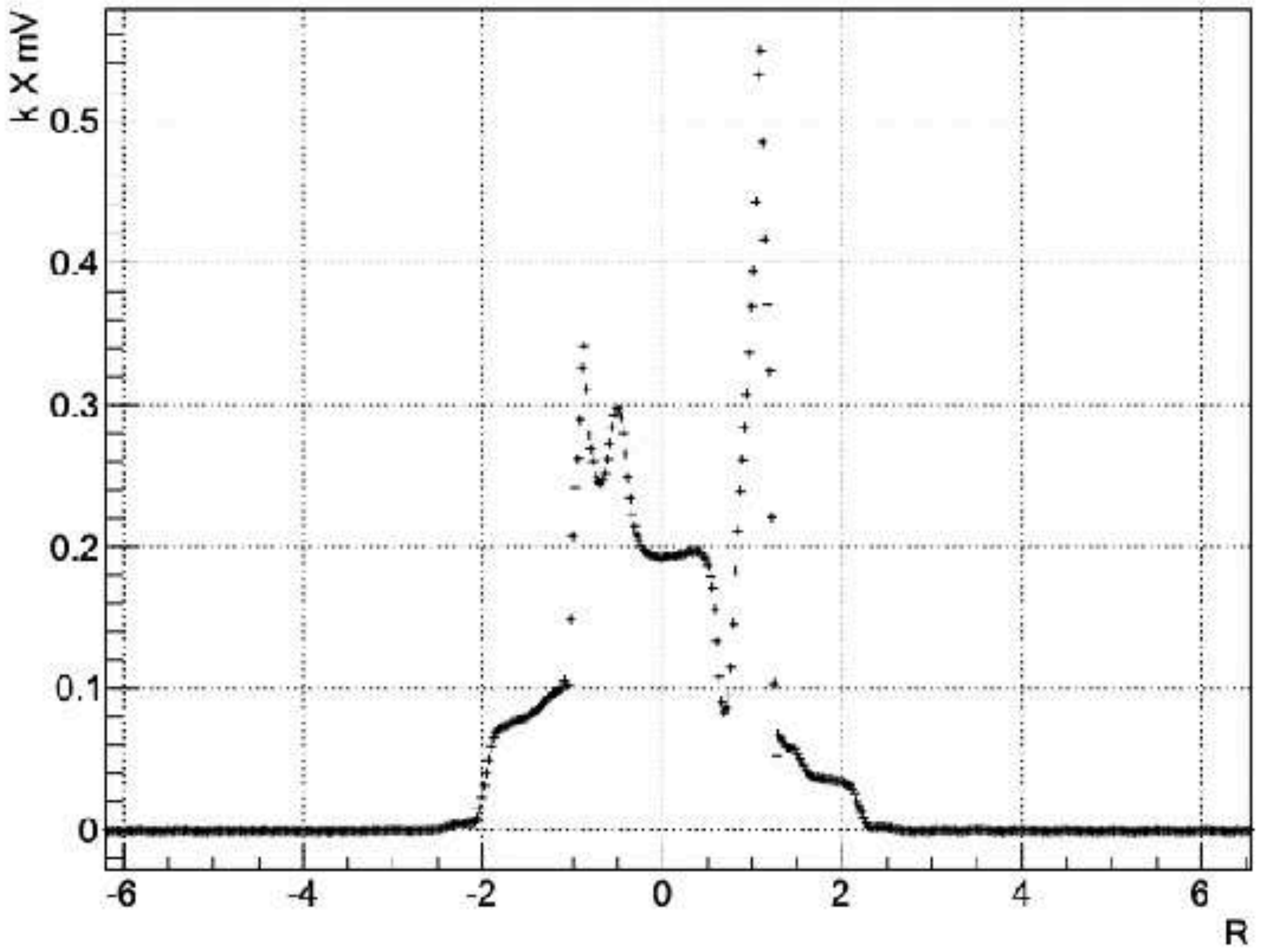

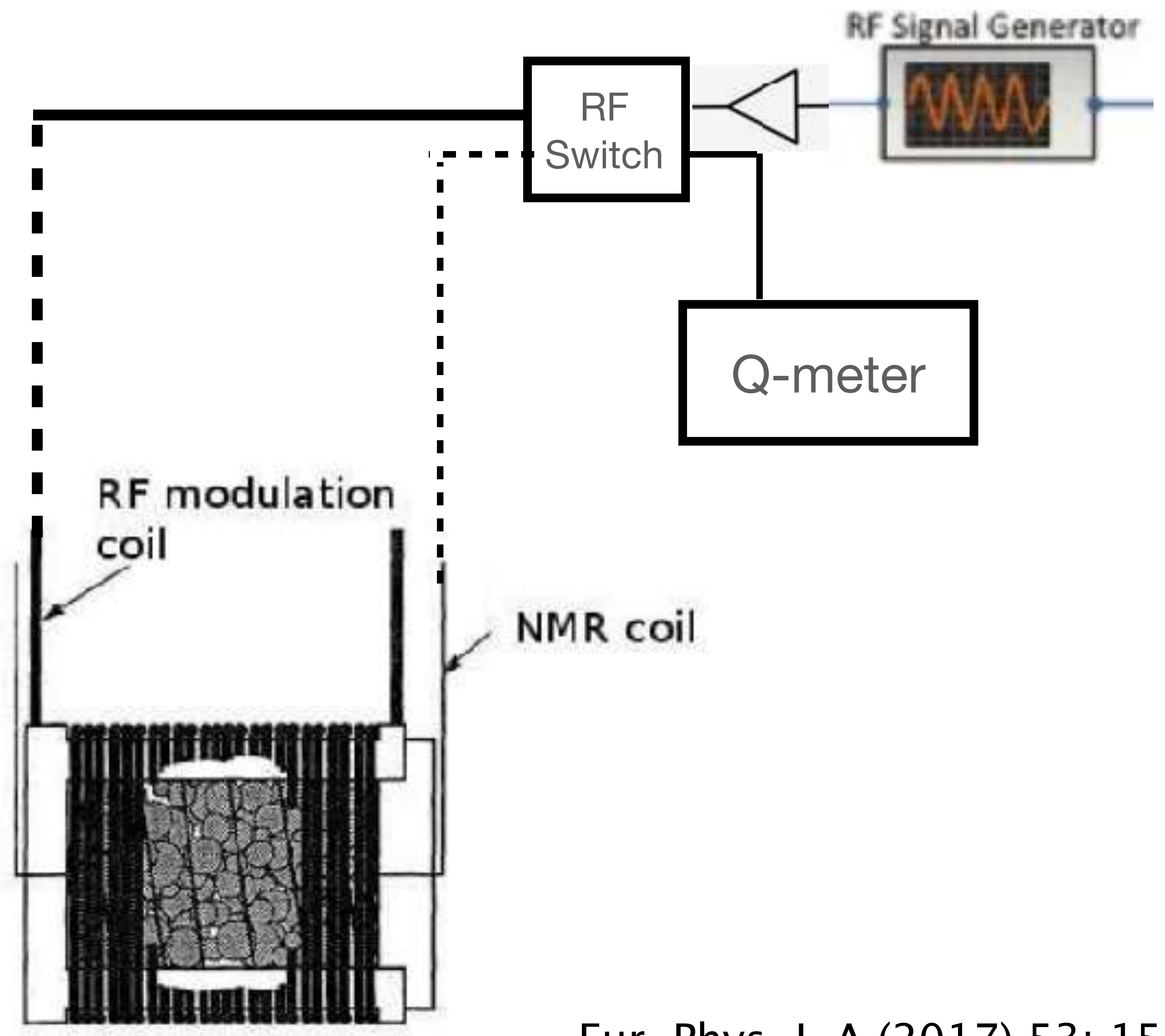

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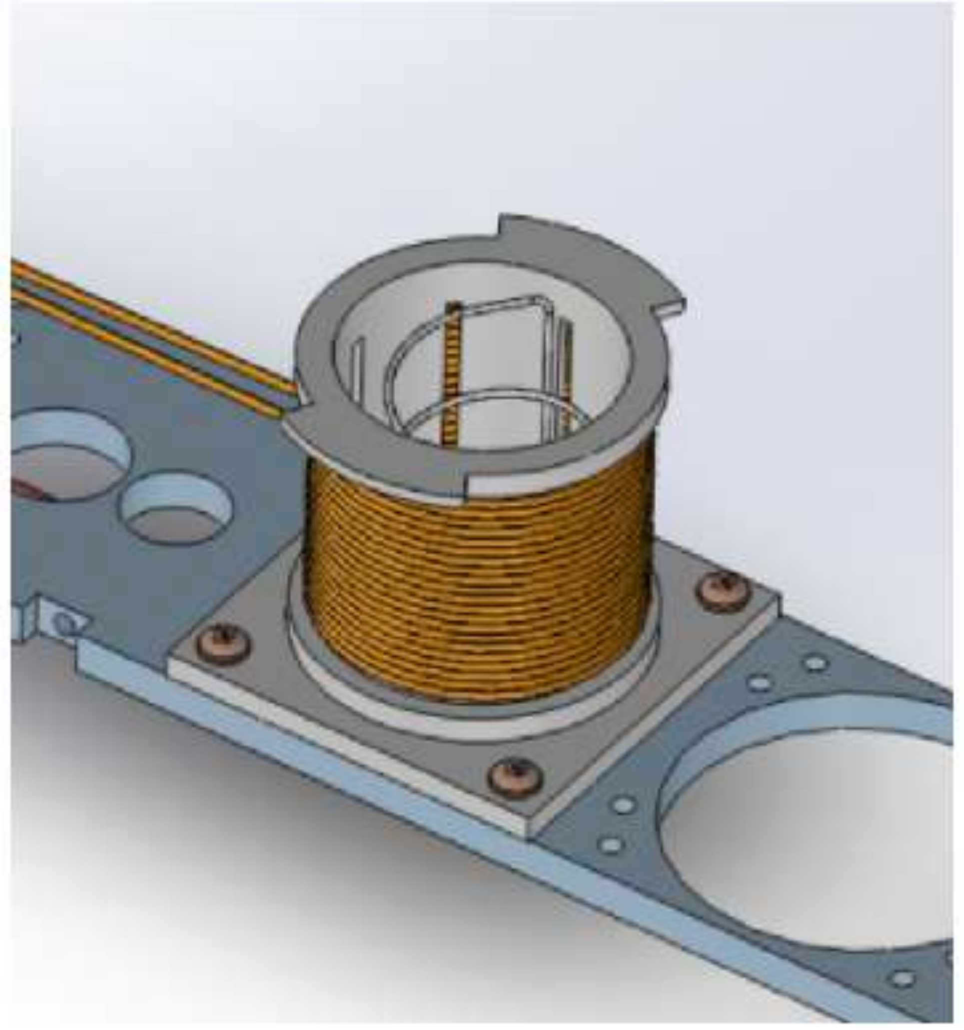
Application of RF

In Selective Semi-saturation



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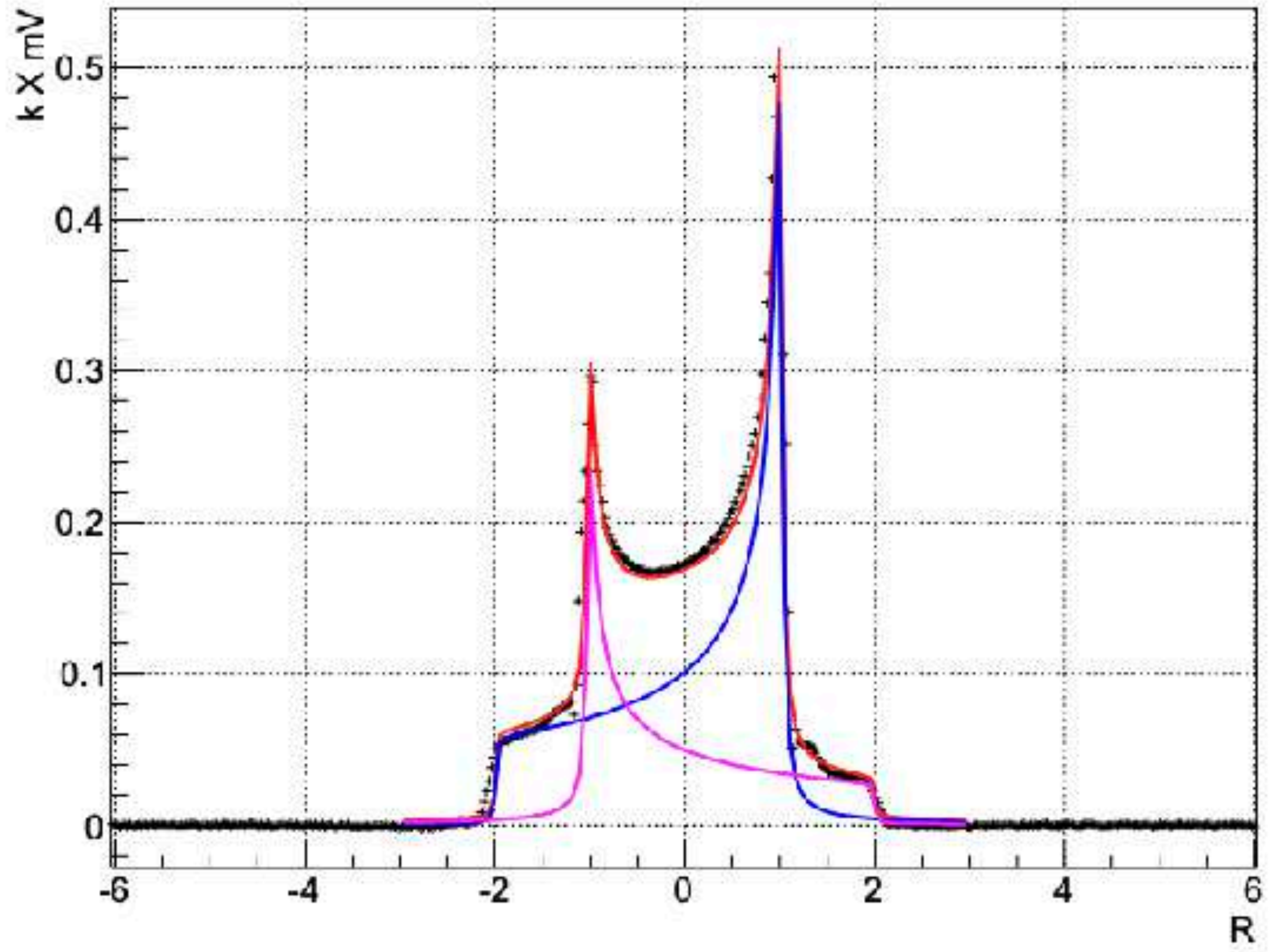

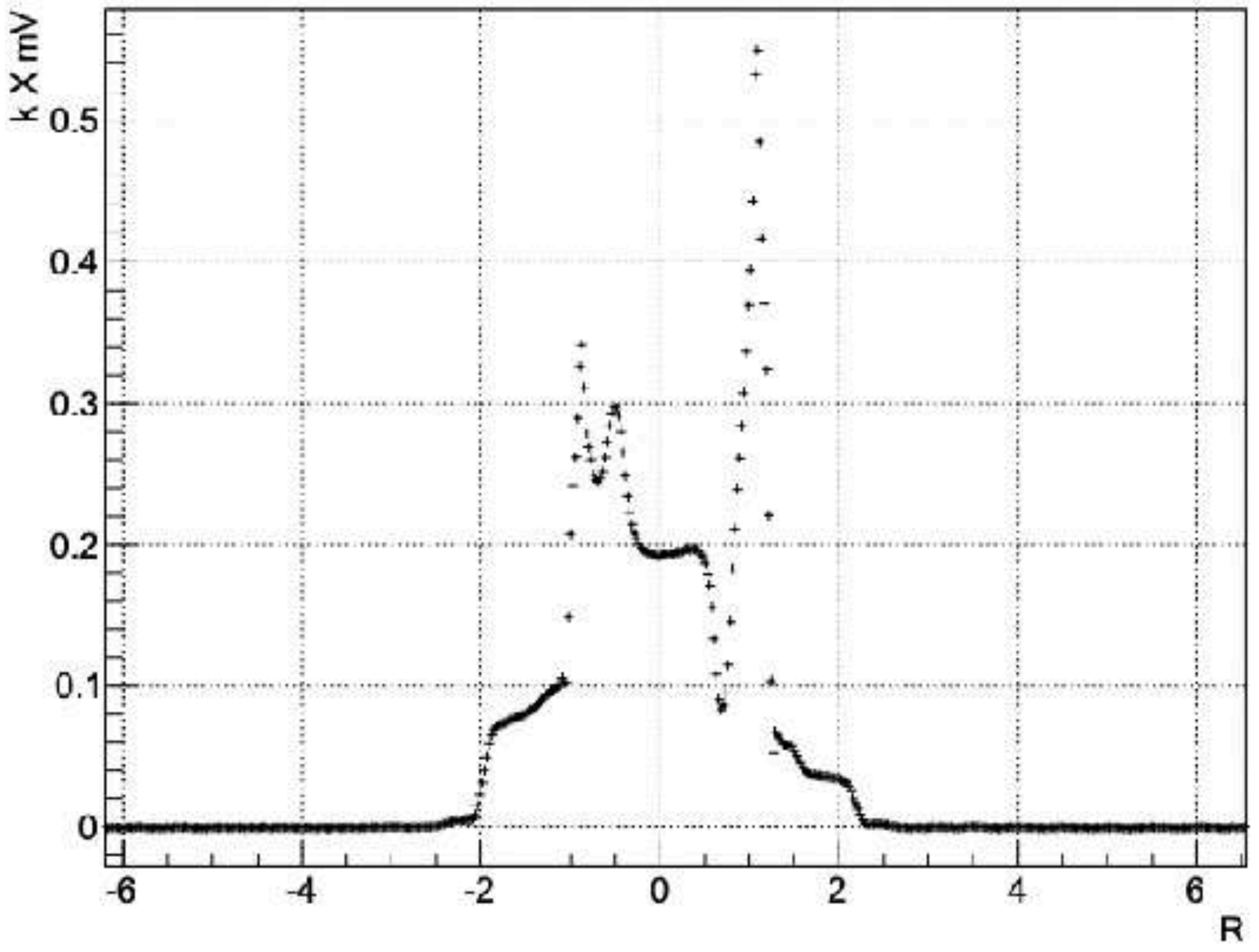

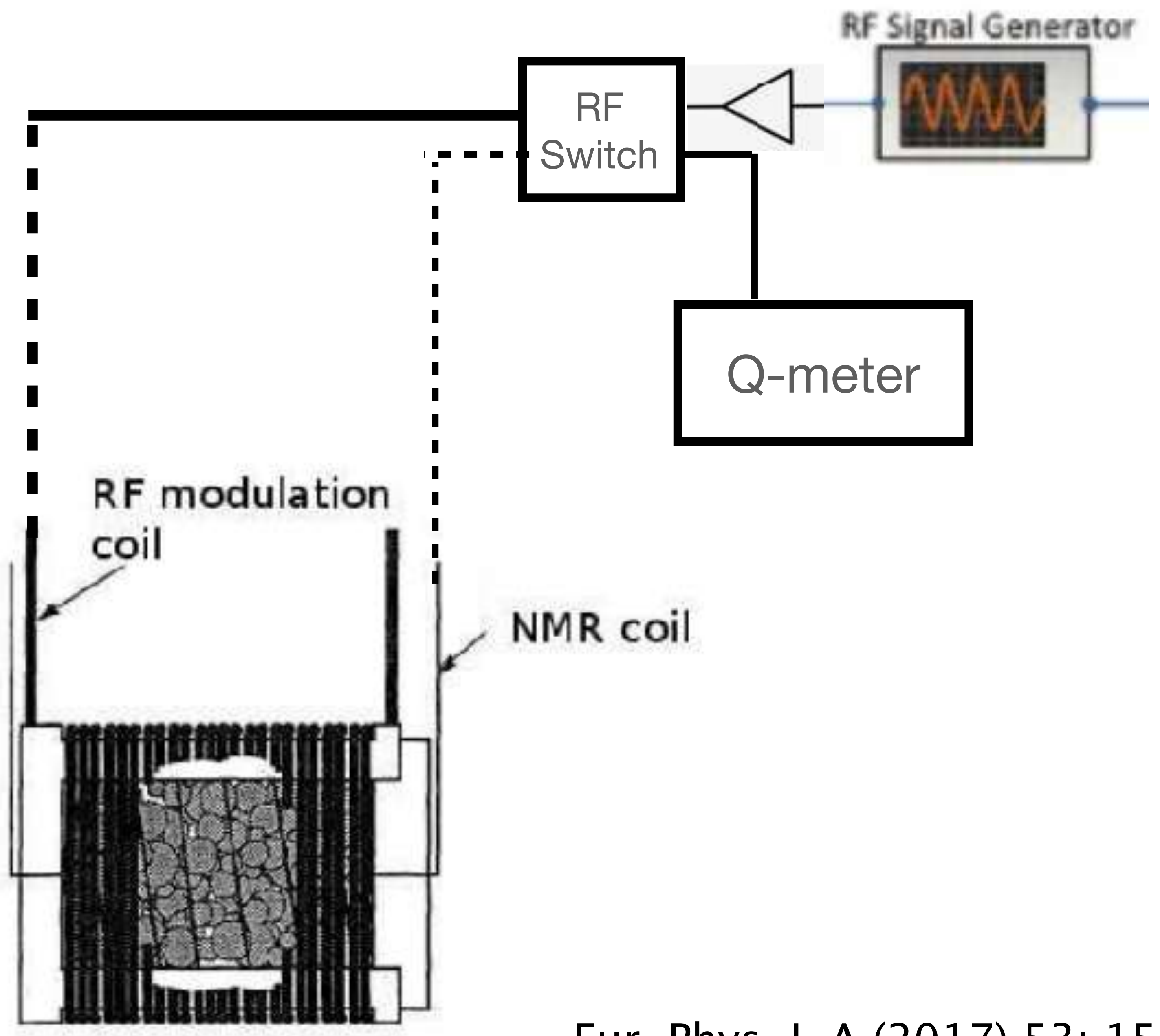

To enhance tensor polarization we must maximize the difference in I_+ *and* I_-

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Charge-2

How to Measure and What is the Error

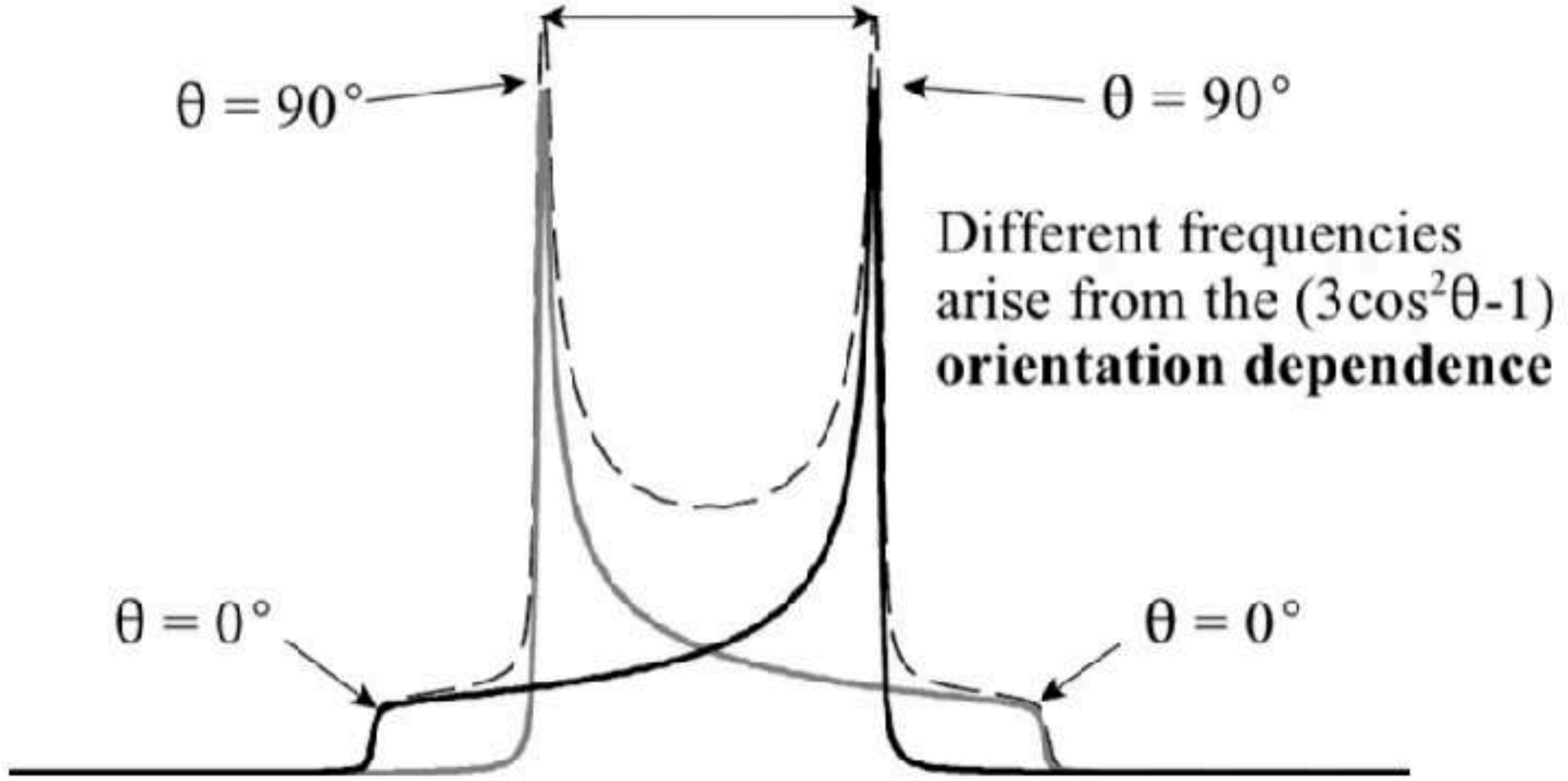
- Measure
  - Assume TE and Boltzmann signal studies well during calibration
  - Use 3-principle extraction
  - Continue to sweep-measure/sweep-manipulate
- Uncertainty
  - Additional Error from modulating but have tools to improve

The Three Essential Concepts

For Enhanced Tensor Polarization that can be measured

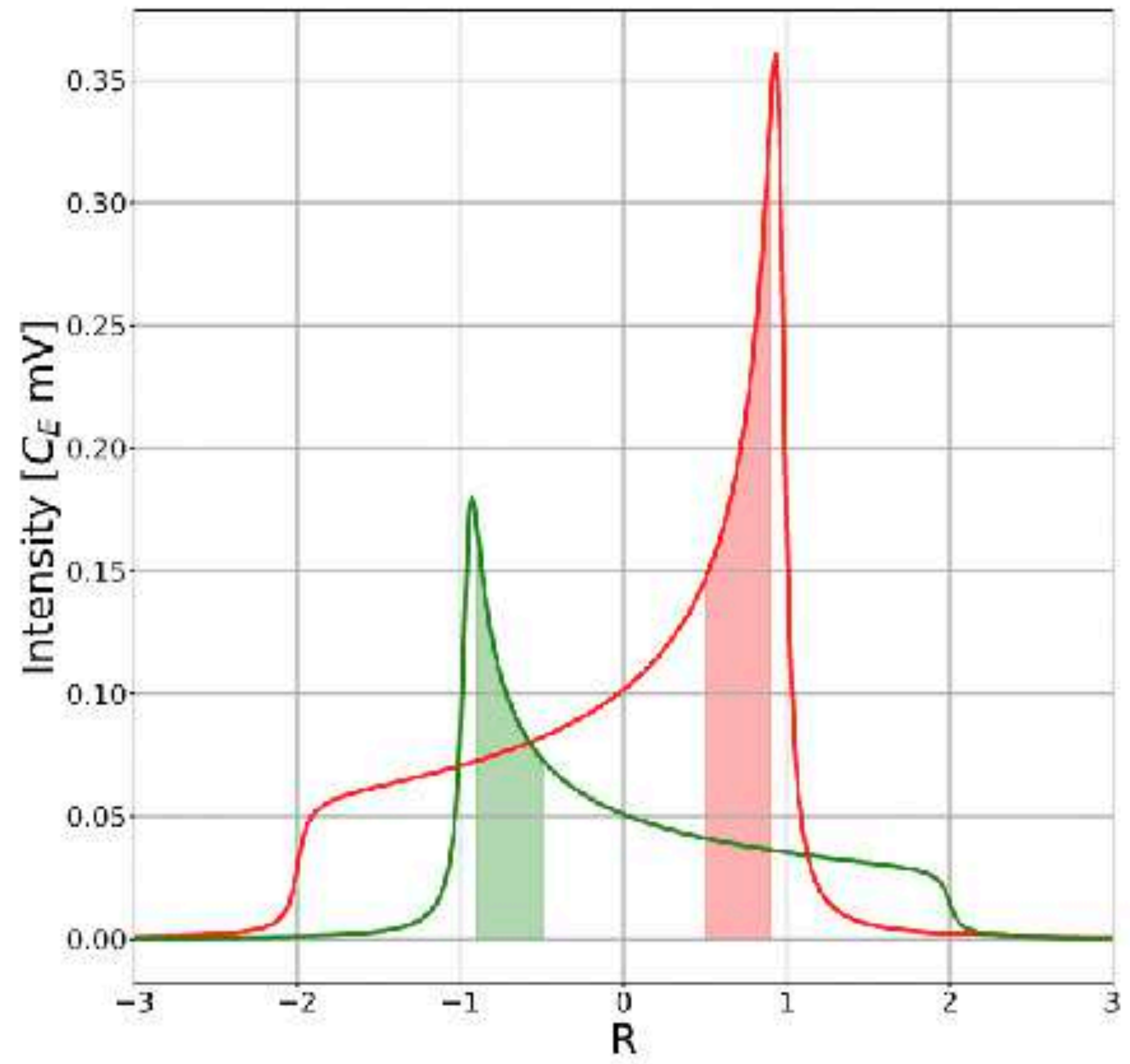
- Differential Binning
- Spin Temperature Consistency
- Rates Response

\



Different frequencies arise from the ($3\cos^2\theta$-1) **orientation dependence**

Differential Binning



$$P = C(I_+ + I_-)$$

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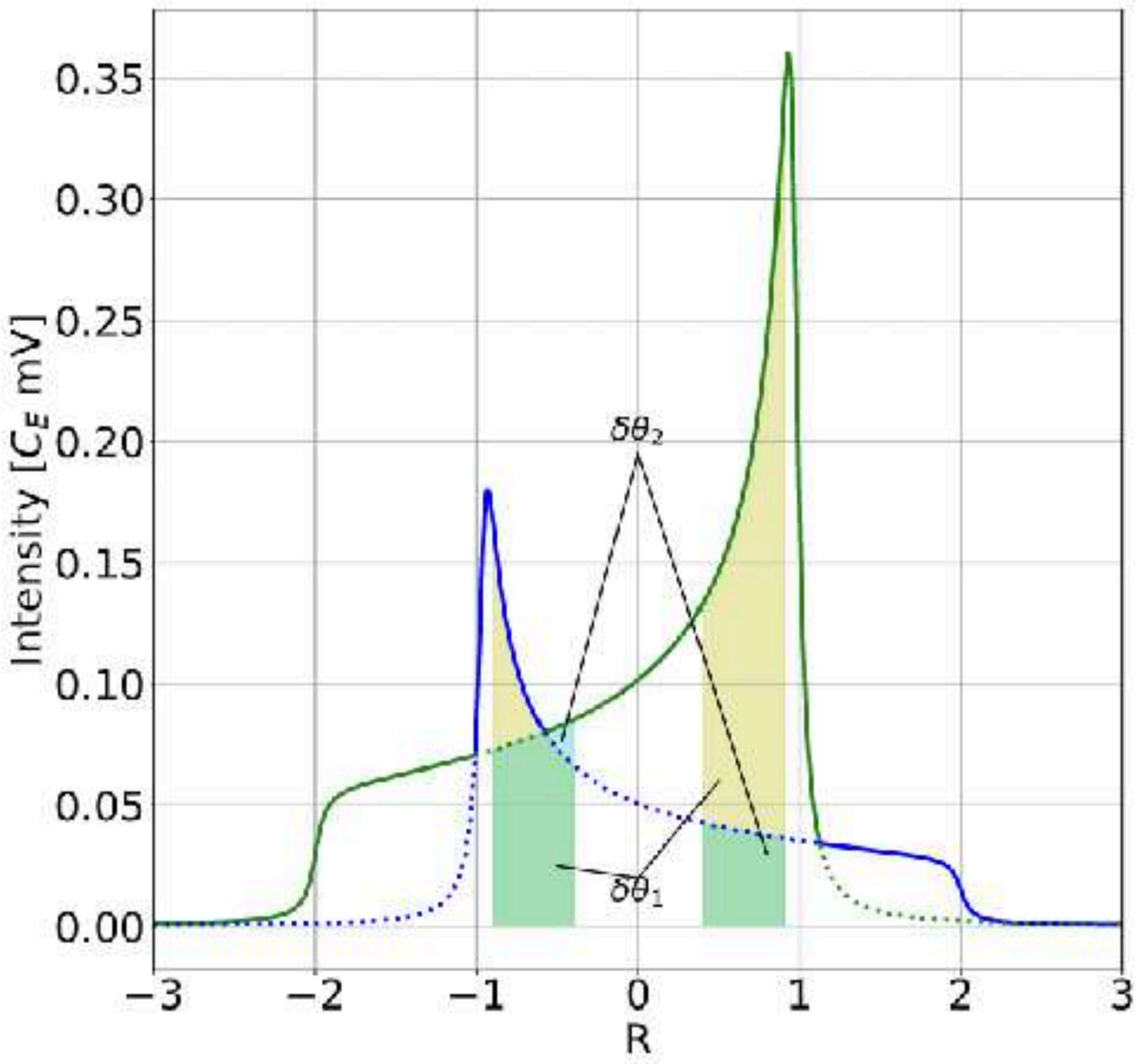
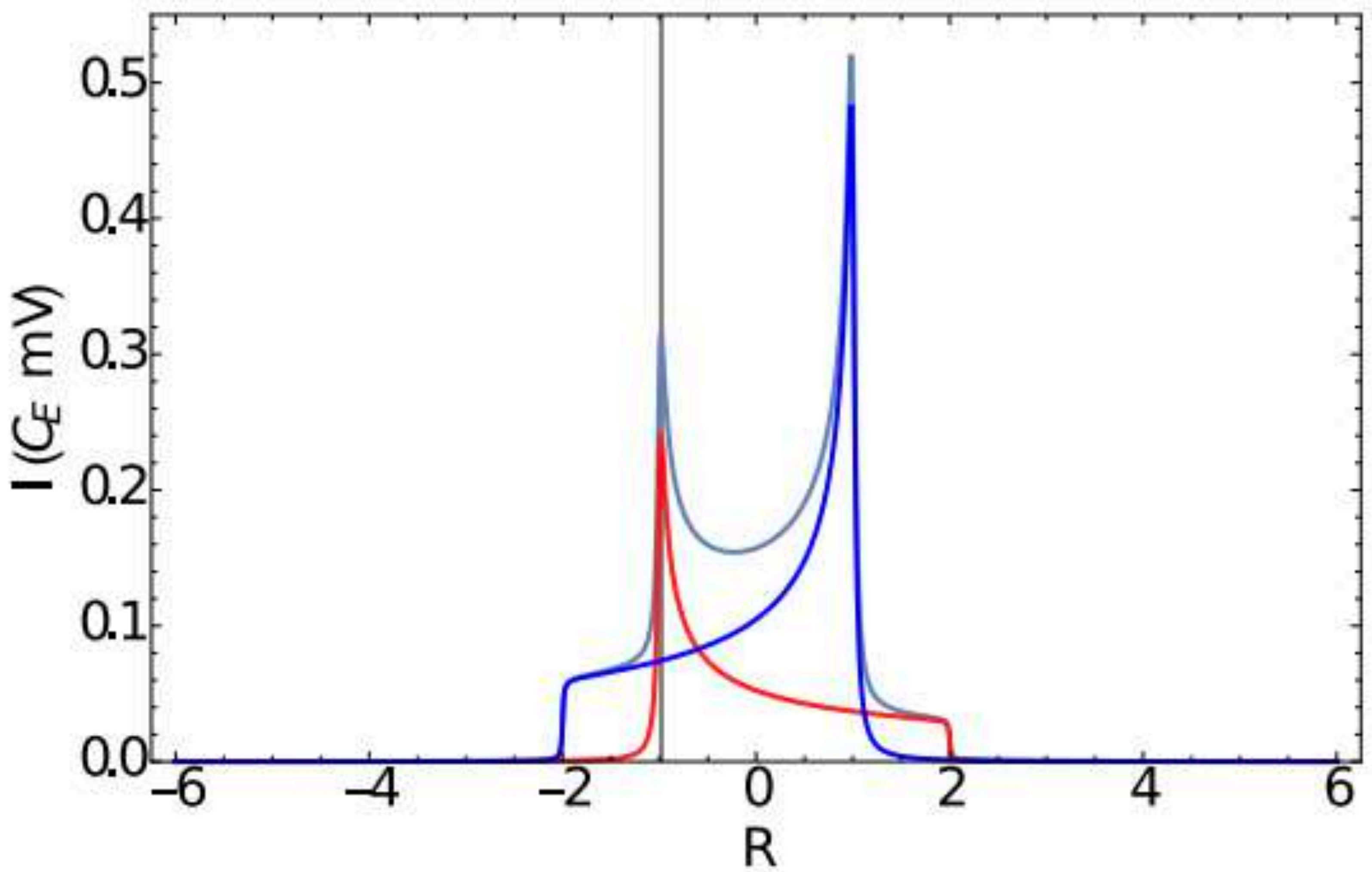
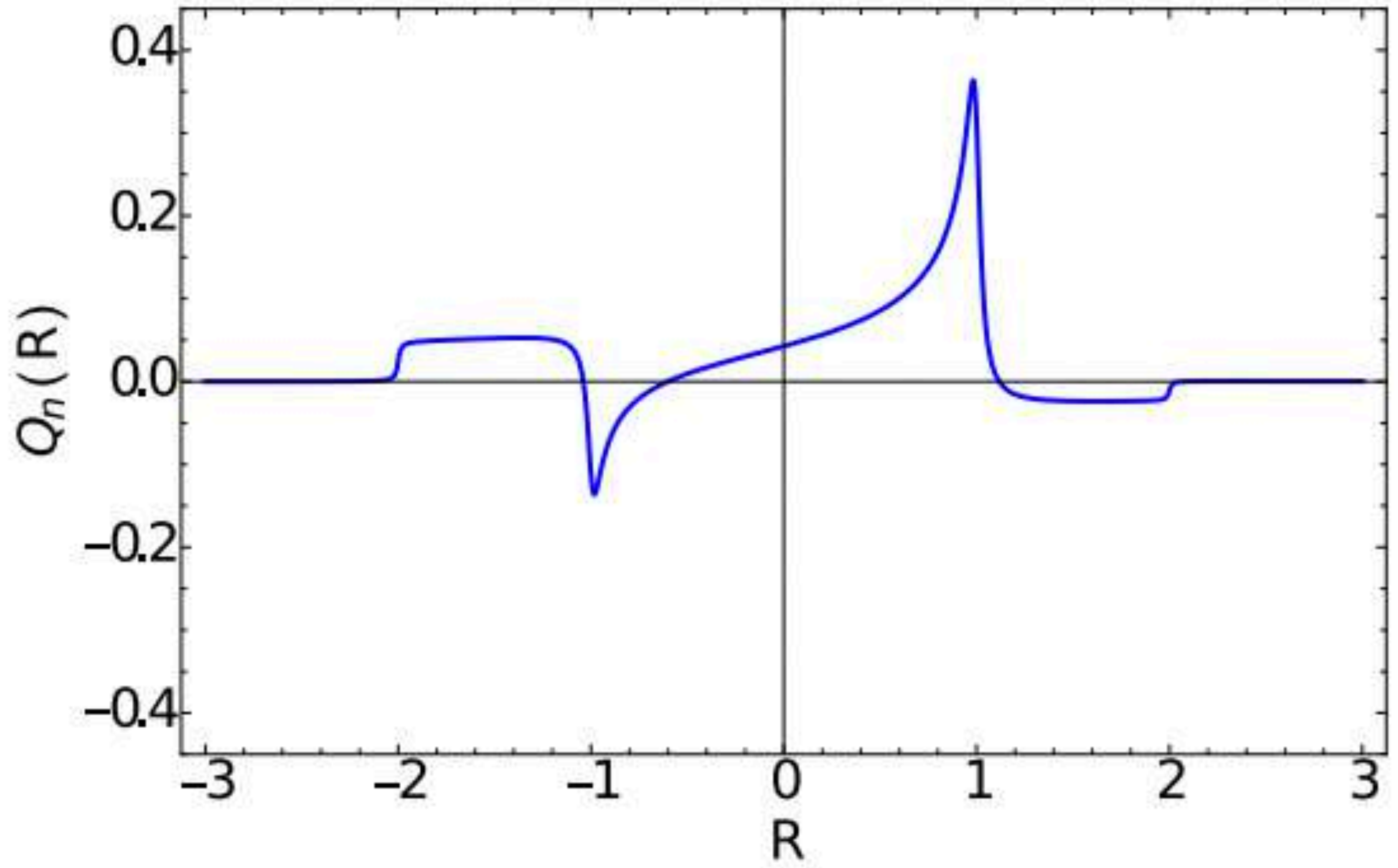


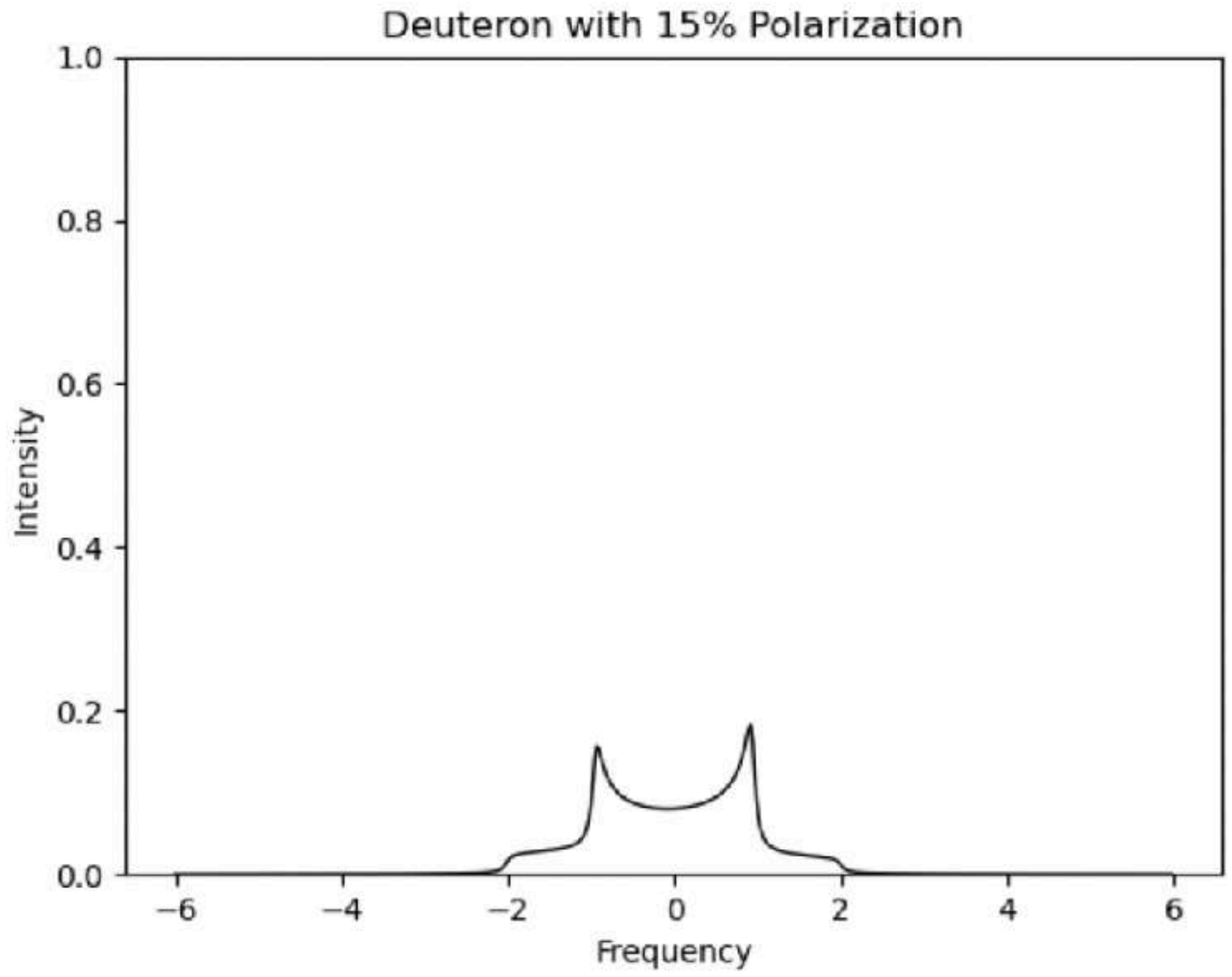


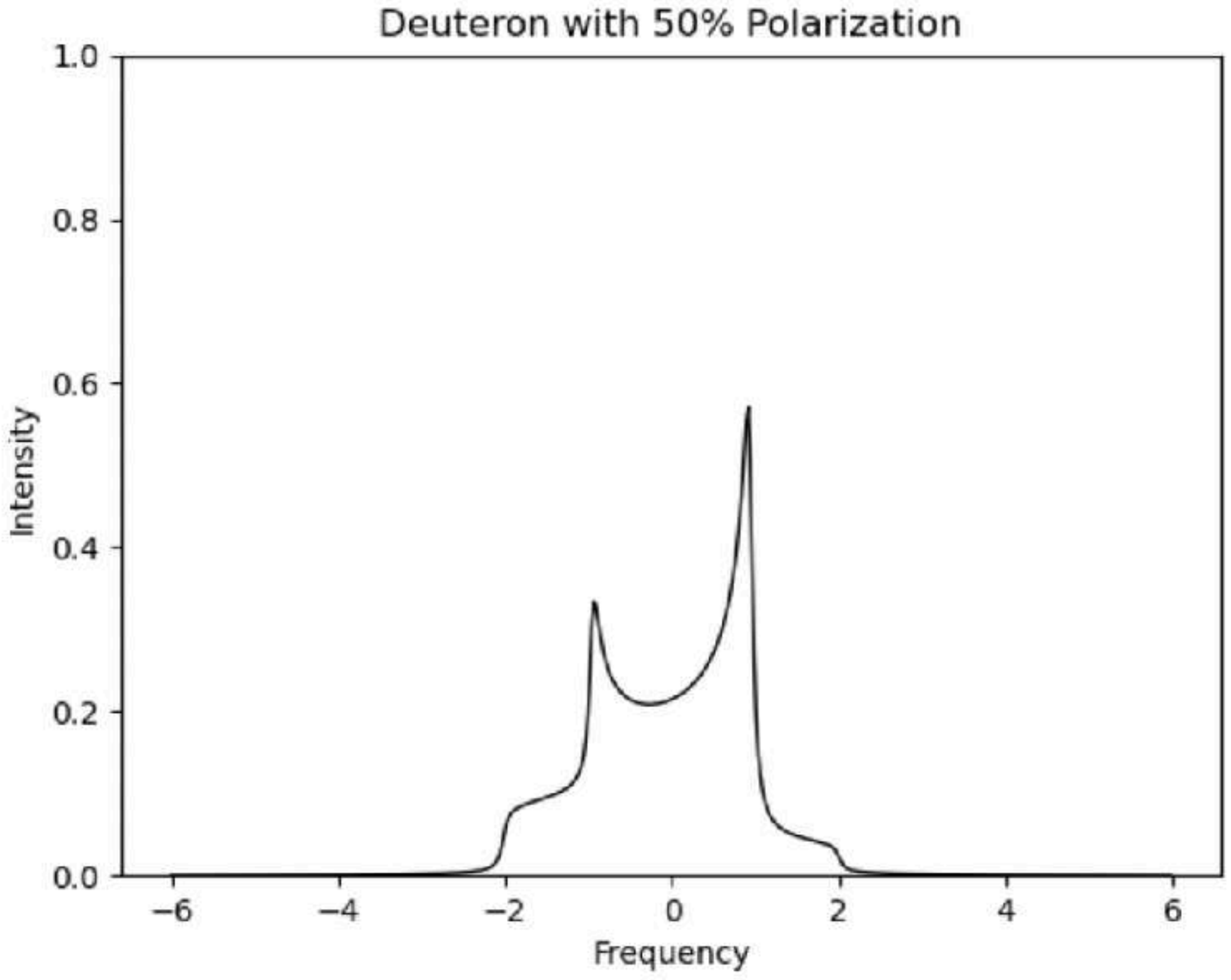
Depolarized back to zero



Spin Temperature Consistency

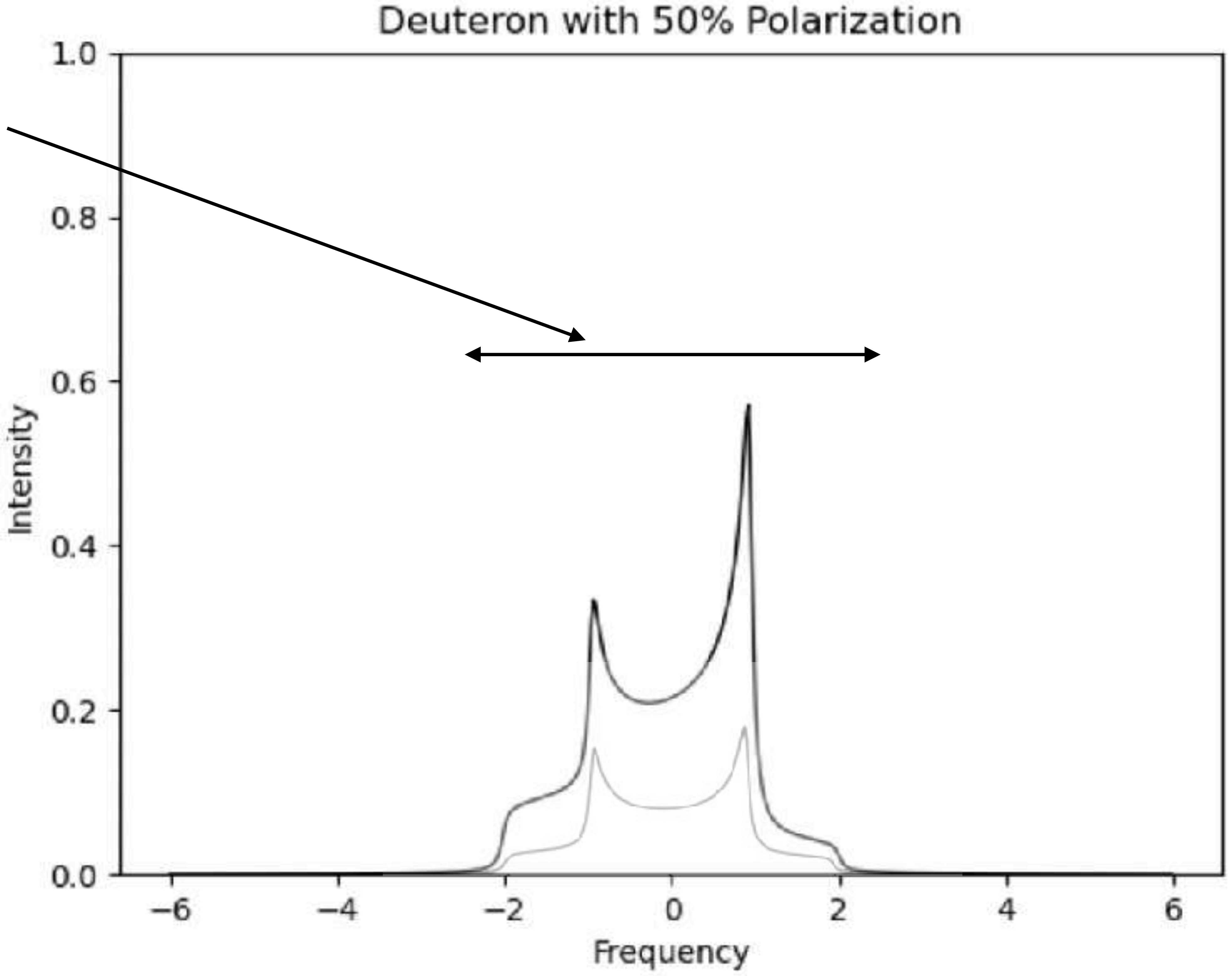
or strategic depolarization





Spin Temperature Consistency
or strategic depolarization

Applying saturating or semi-saturating RF
Can only ever depolarize

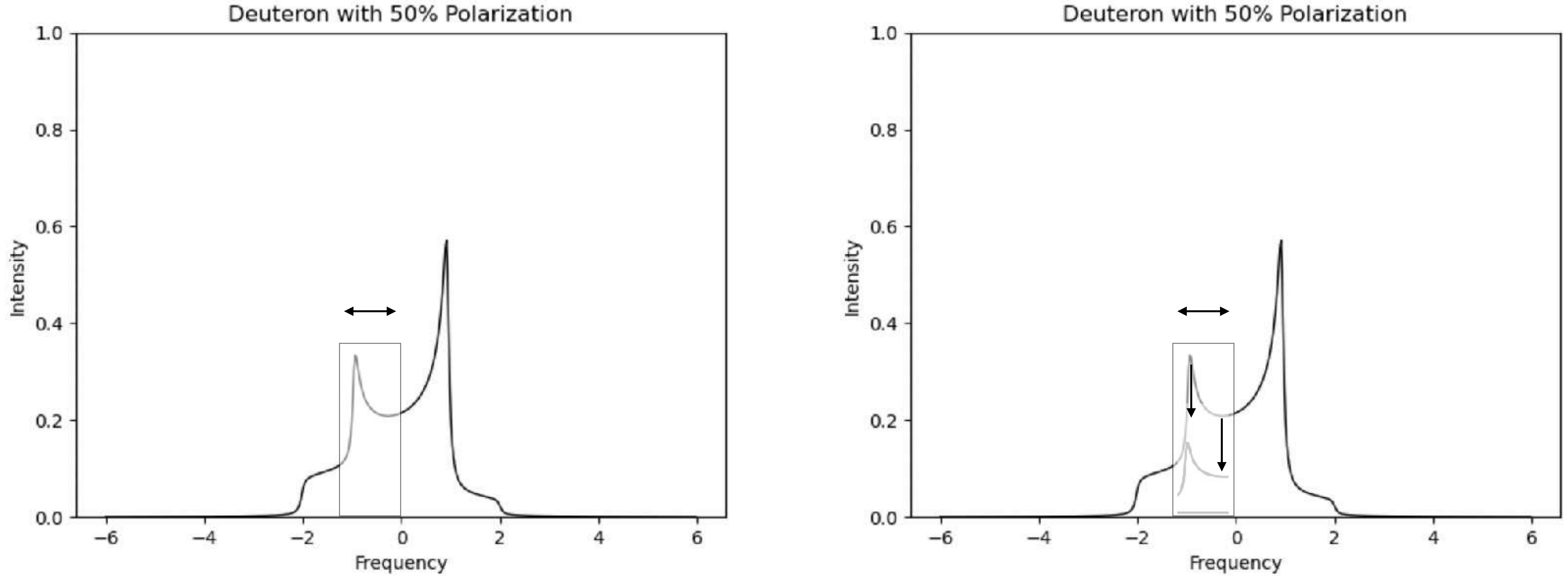


$$\omega_m \gg 2\pi/T_1$$

Fast enough that we treat this
As the application of a homogeneous field

Spin Temperature Consistency

or strategic depolarization



Spin Temperature Consistency

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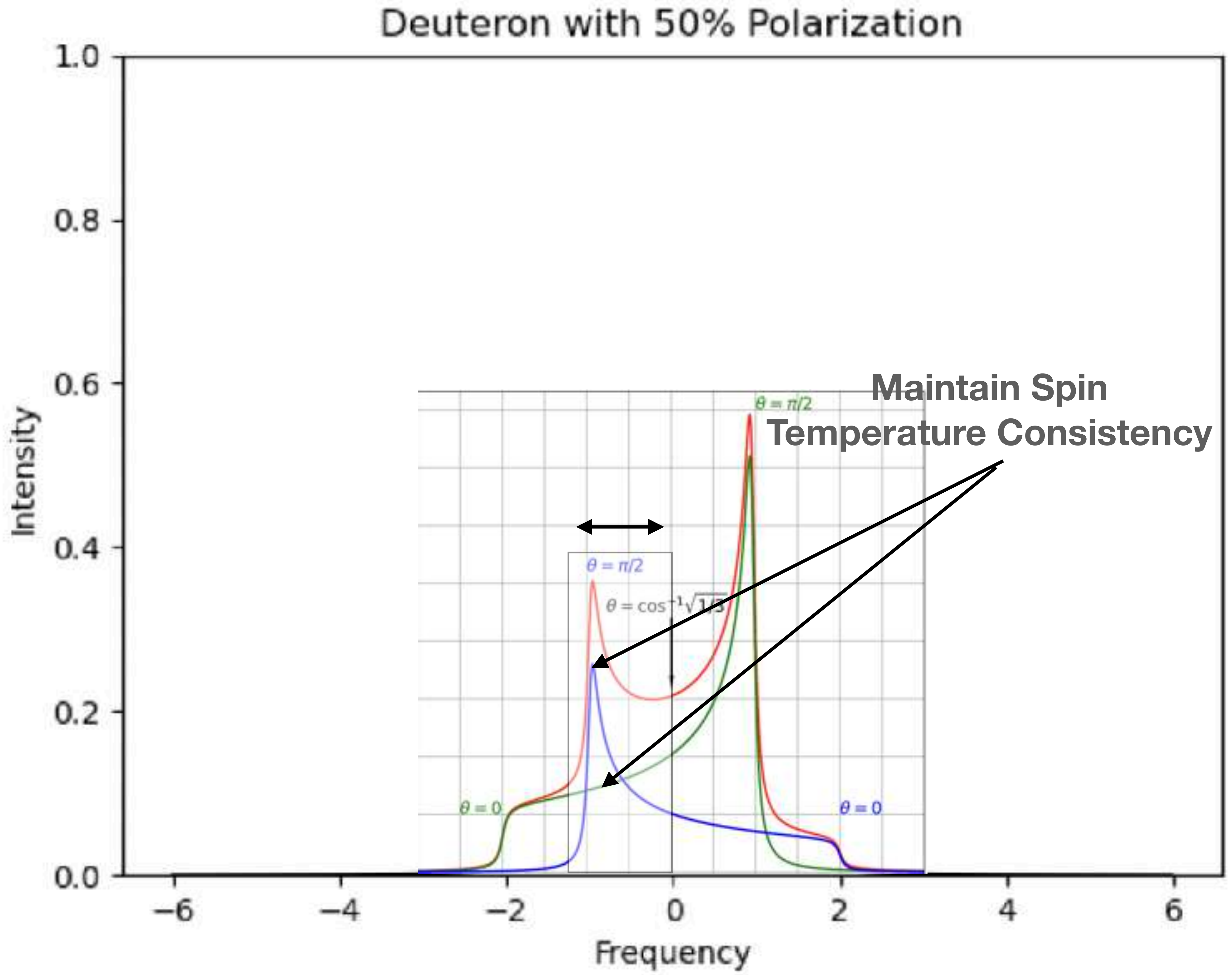
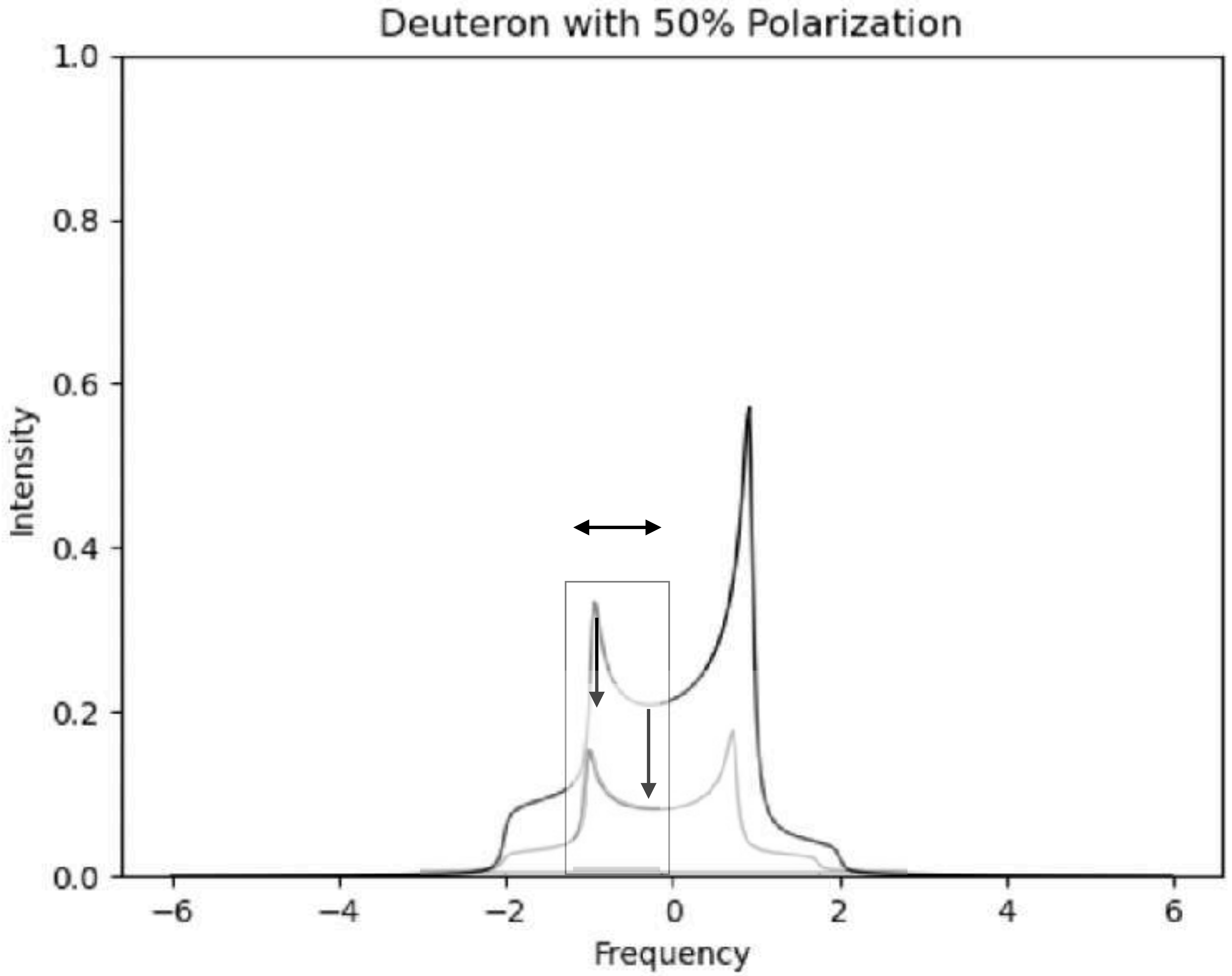


Maintain Spin Temperature Consistency

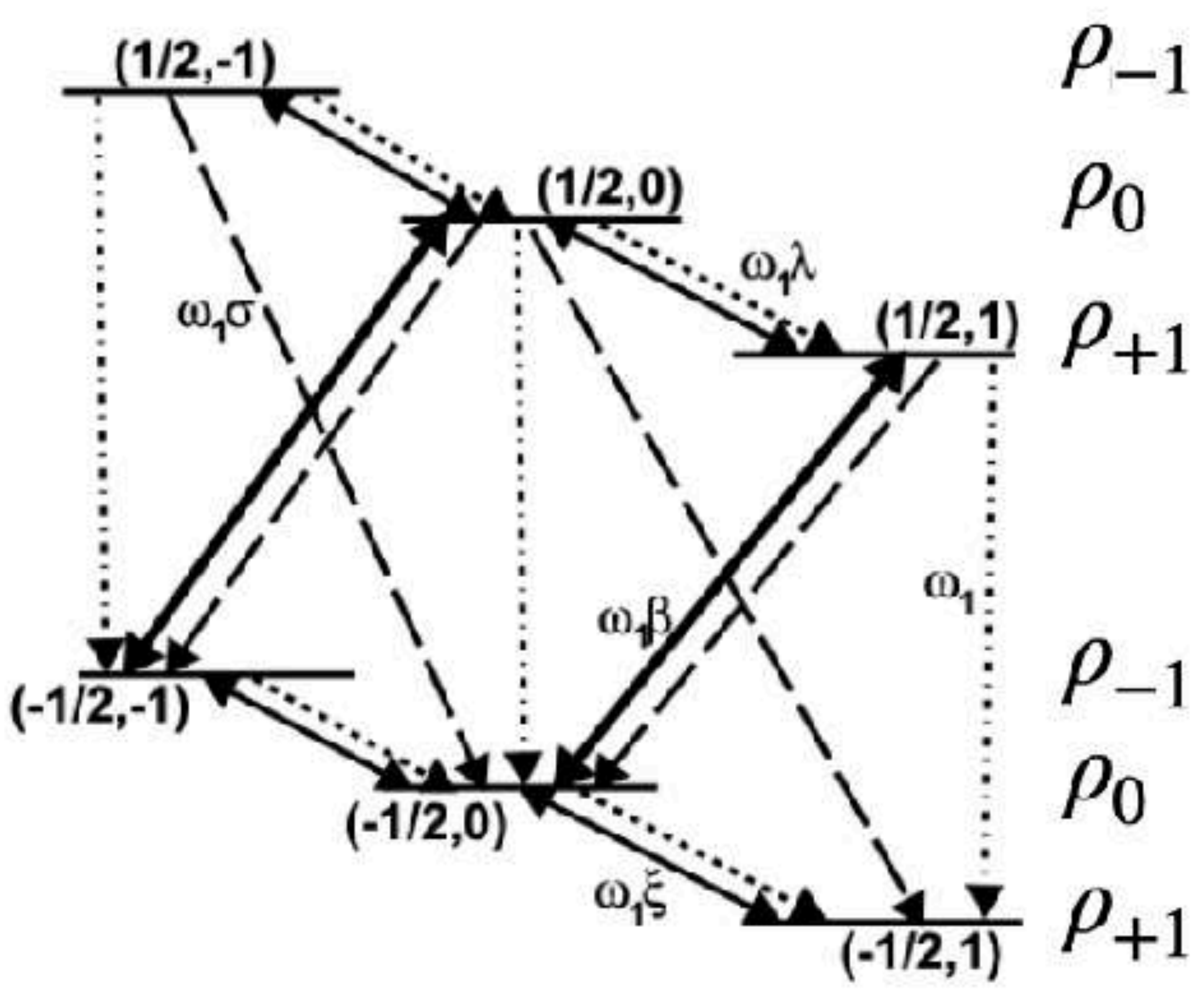


Principle: If you know the sum you know the difference

Rate Response

Or why you can get rid of models

$$A_{lost} = \frac{1}{2}A_{gained}$$



$$I_- = C(\rho_0 - \rho_-)$$

$$\dot{I}_-(-\mathscr{R}) = C\left[\dot{\rho}_0(-\mathscr{R}) - \dot{\rho}_-(-\mathscr{R})\right]$$

$$\dot{\rho}_0(-\mathscr{R}) = -\xi\rho_0(-\mathscr{R}) + \xi\rho_-(-\mathscr{R})$$

$$\dot{\rho}_-(-\mathscr{R}) = -\xi\rho_-(-\mathscr{R}) + \xi\rho_0(-\mathscr{R})$$

$$I_+ = C(\rho_+ - \rho_0)$$

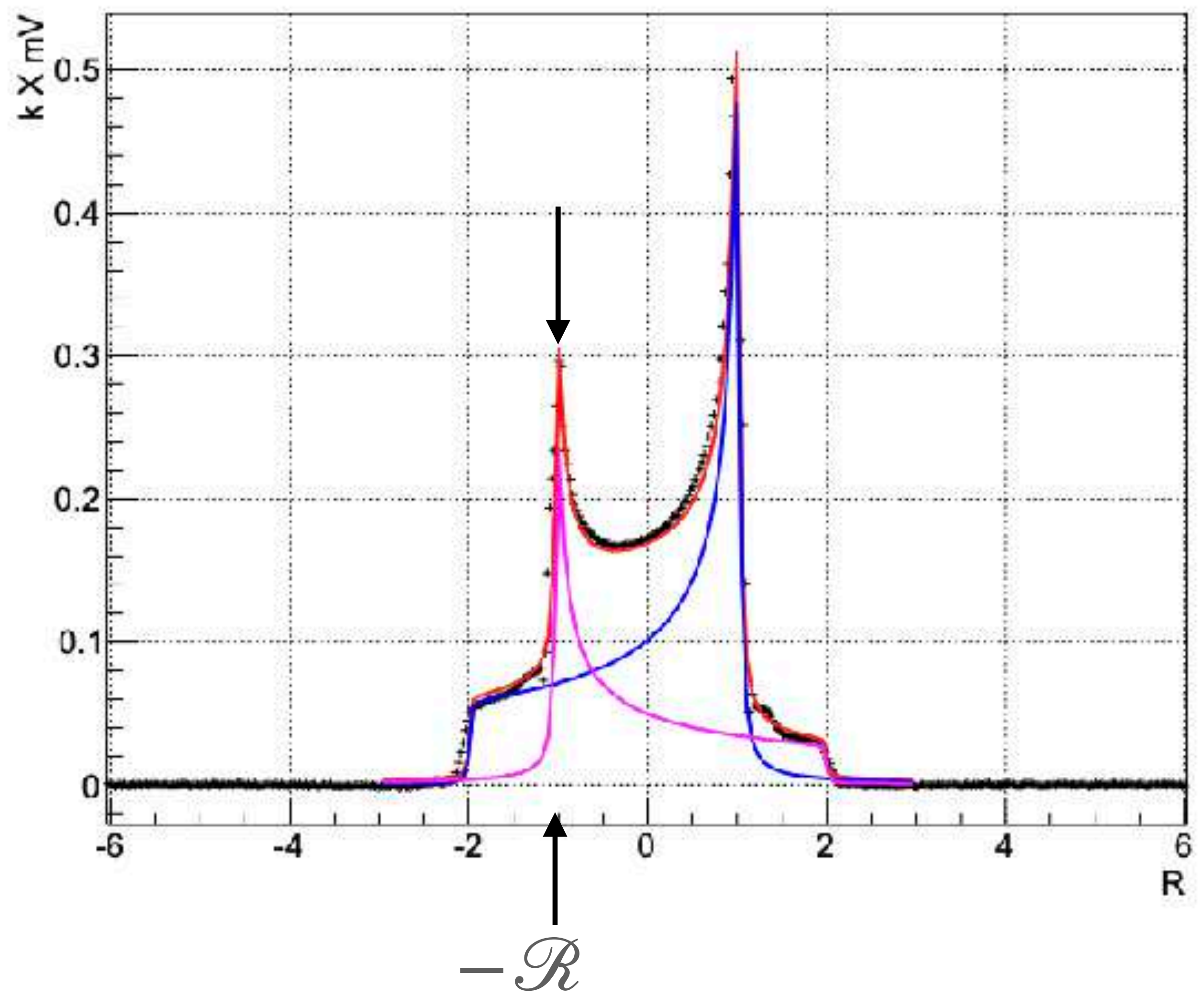
$$\dot{I}_+(-\mathscr{R}) = C\left[\dot{\rho}_+(-\mathscr{R}) - \dot{\rho}_0(-\mathscr{R})\right]$$

$$\dot{\rho}_+(-\mathscr{R}) = -\xi\rho_+(-\mathscr{R}) + \xi\rho_0(-\mathscr{R}$$

$$\dot{\rho}_0(-\mathscr{R}) = -\xi\rho_0(-\mathscr{R}) + \xi\rho_+(-\mathscr{R})$$

$$\begin{aligned}\dot{I}_-(-\mathscr{R}) &= C\left[\dot{\rho}_0(-\mathscr{R}) - \dot{\rho}_-(-\mathscr{R})\right]\\ &= -\xi\left[\rho_0(-\mathscr{R}) - \rho_-(-\mathscr{R})\right]\\ &\quad +\xi\left[\rho_-(-\mathscr{R}) - \rho_0(-\mathscr{R})\right]\\ &= -2\xi I_-(-\mathscr{R})\end{aligned}$$

$$\begin{aligned}\dot{I}_+(-\mathscr{R}) &= C\left[\dot{\rho}_0(-\mathscr{R}) - \dot{\rho}_-(-\mathscr{R})\right]\\ &= -\xi\left[\rho_+(-\mathscr{R}) - \rho_0(-\mathscr{R})\right]\\ &\quad +\xi\left[\rho_0(-\mathscr{R}) - \rho_+(-\mathscr{R})\right]\\ &= -2\xi I_+(-\mathscr{R})\end{aligned}$$



Rate Response

Or why you can get rid of models

$$I_+ = C(\rho_+ - \rho_0)$$

$$\dot{I}_+(\mathscr{R}) = C\left[\dot{\rho}_+(\mathscr{R}) - \dot{\rho}_0(\mathscr{R})\right]$$

$$\dot{\rho}_+(\mathscr{R}) = \xi\rho_+(\mathscr{R}) - \xi\rho_0(\mathscr{R})$$

$$\dot{\rho}_0(\mathscr{R}) = \xi\rho_0(\mathscr{R}) - \xi\rho_+(\mathscr{R})$$

$$\begin{aligned}\dot{I}_+(\mathscr{R}) &= C\left[\dot{\rho}_+(\mathscr{R}) - \dot{\rho}_0(\mathscr{R})\right]\\ &= -\,\xi\dot{\rho}_0(\mathscr{R})\\ &= -\,\xi\left[\rho_0(\mathscr{R}) - \rho_+(\mathscr{R})\right]\\ &= \xi I_+(\mathscr{R})\end{aligned}$$

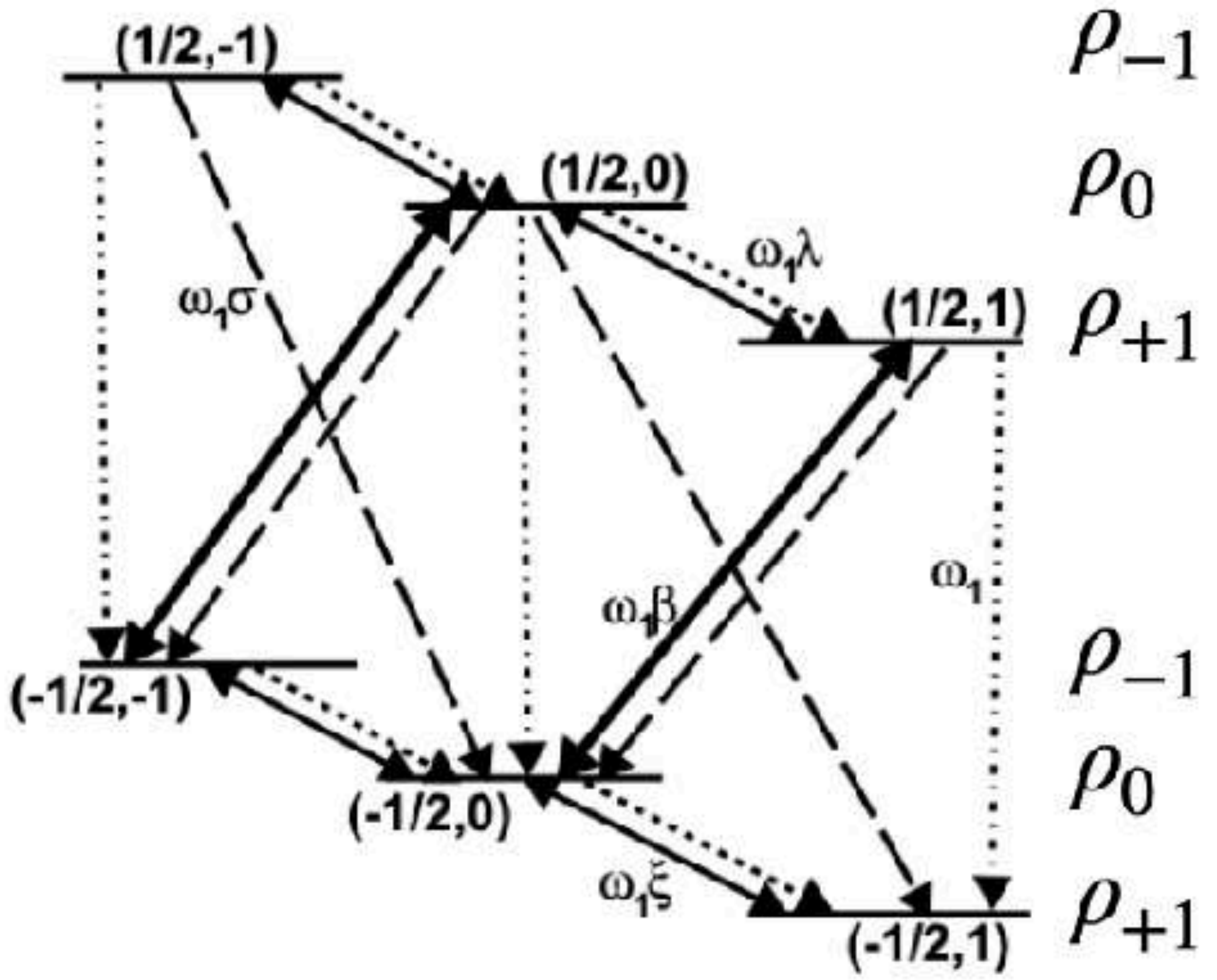
$$I_- = C(\rho_0 - \rho_-)$$

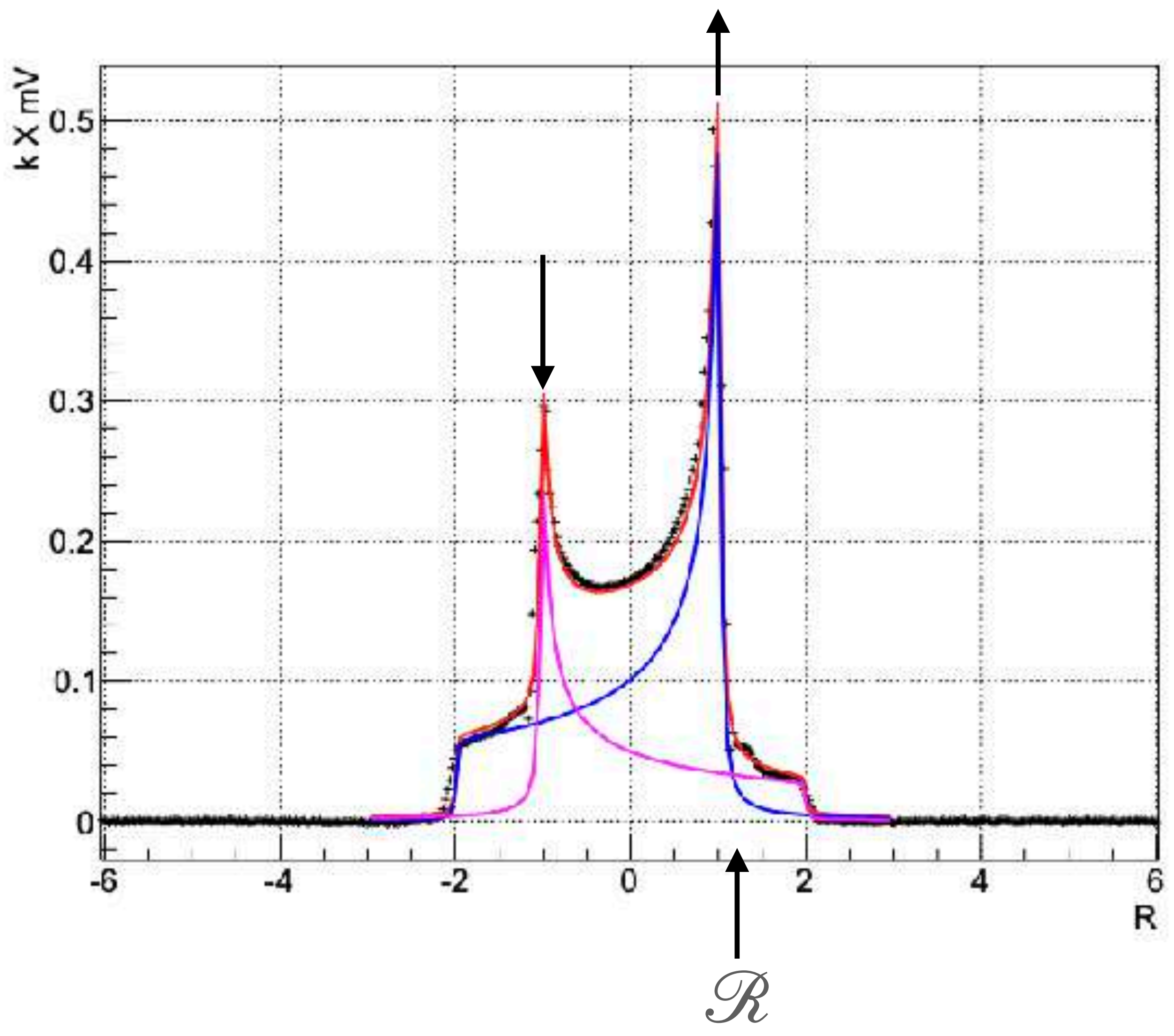
$$\dot{I}_-(\mathscr{R}) = C\left[\dot{\rho}_0(\mathscr{R}) - \dot{\rho}_-(\mathscr{R})\right]$$

$$\dot{\rho}_0(\mathscr{R}) = \xi\rho_0(\mathscr{R}) - \xi\rho_-(\mathscr{R})$$

$$\dot{\rho}_-(\mathscr{R}) = \xi\rho_-(\mathscr{R}) - \xi\rho_0(\mathscr{R})$$

$$\begin{aligned}\dot{I}_-(\mathscr{R}) &= C\left[\dot{\rho}_0(\mathscr{R}) - \dot{\rho}_-(\mathscr{R})\right]\\ &= -\,\xi\dot{\rho}_-(\mathscr{R})\\ &= -\,\xi\left[\rho_0(\mathscr{R}) - \rho_-(\mathscr{R})\right]\\ &= \xi I_-(\mathscr{R})\end{aligned}$$





Rate Response

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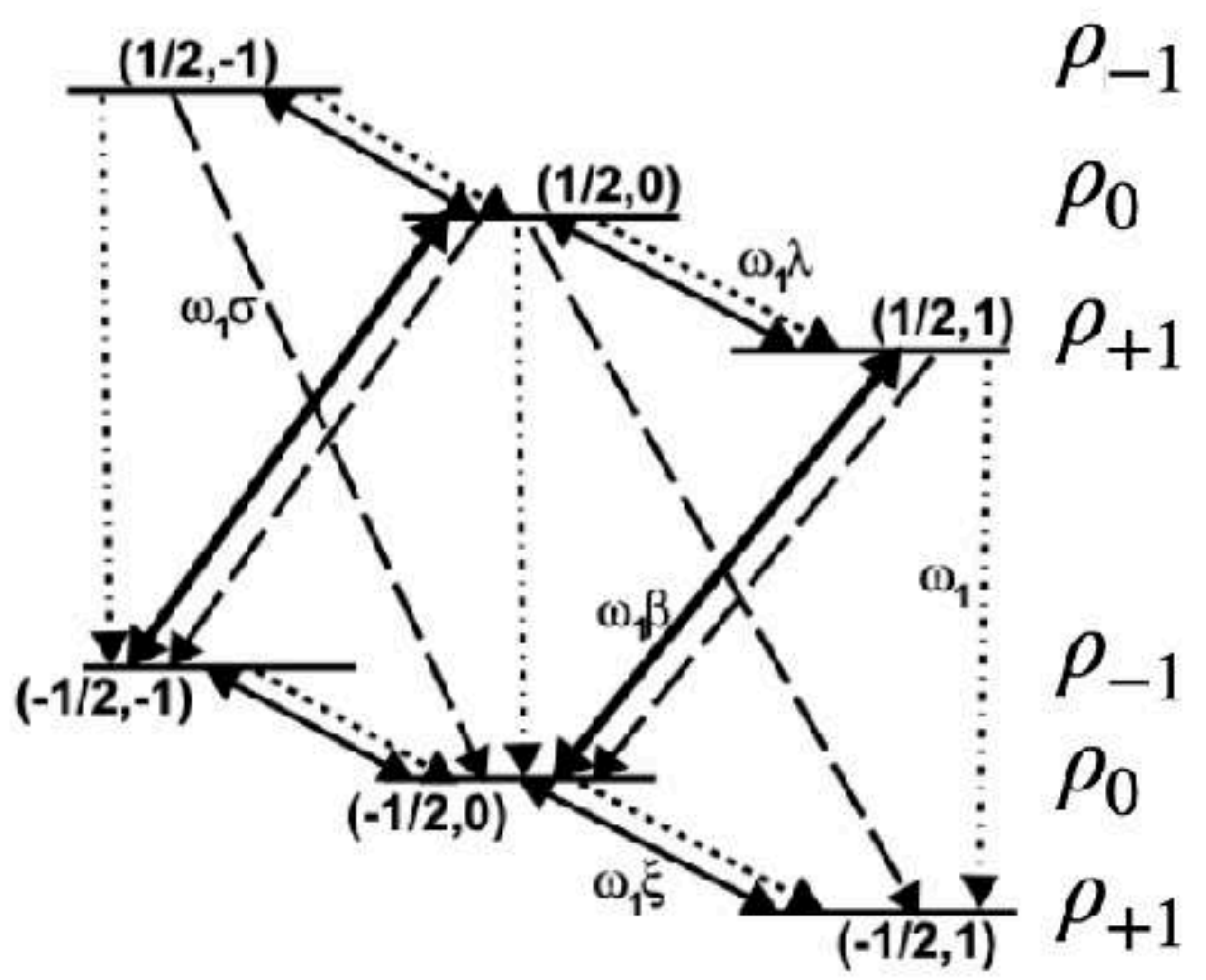
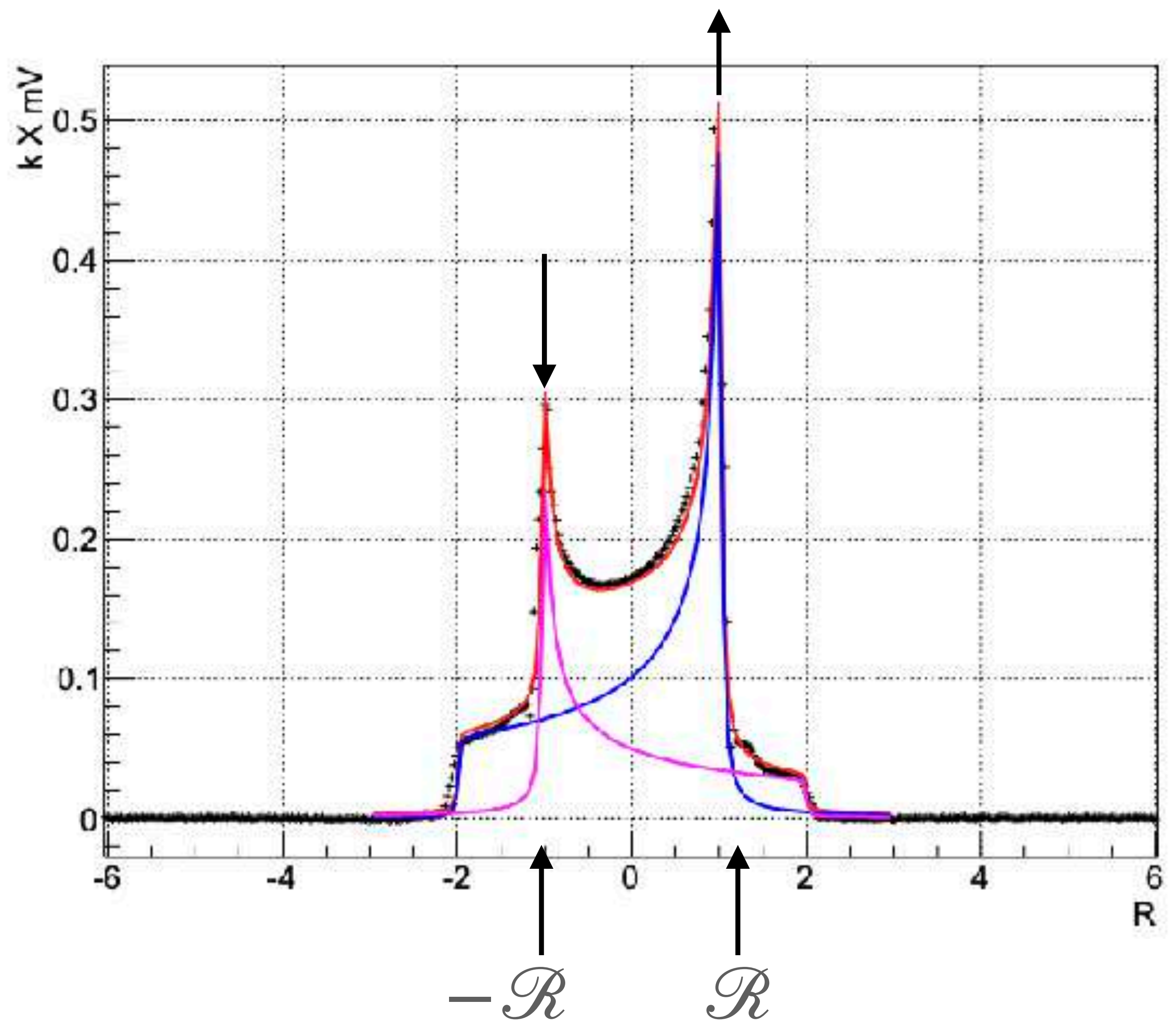


$$\dot{I}_-(-\mathscr{R}) = -2\xi I_-(-\mathscr{R})$$

$$\dot{I}_+(\mathscr{R}) = \xi I_+(\mathscr{R})$$

$$\dot{I}_+(-\mathscr{R}) = -2\xi I_+(-\mathscr{R})$$

$$\dot{I}_-(\mathscr{R}) = \xi I_-(\mathscr{R})$$



$$2A_{lost} = A_{gained}$$

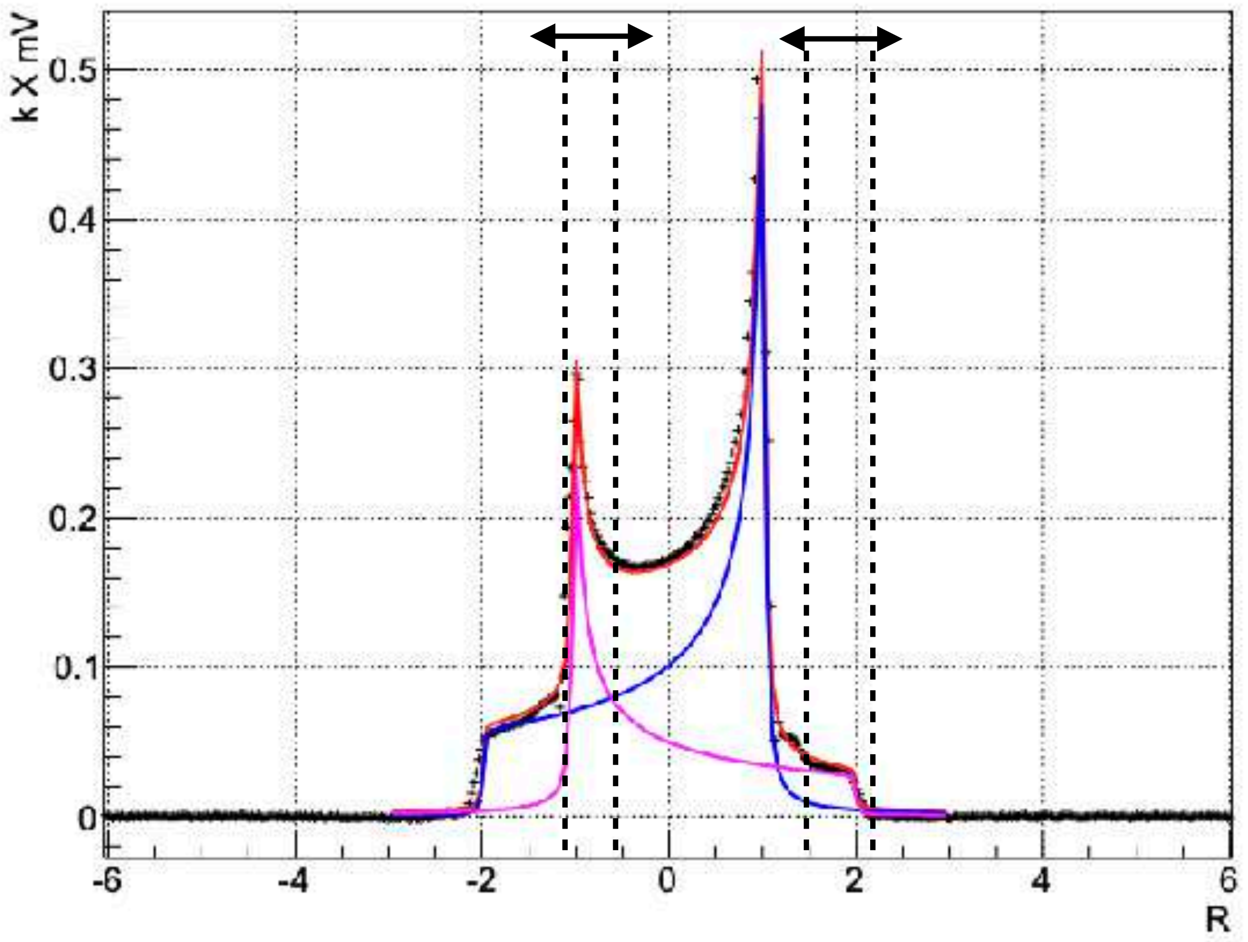
$$\boxed{A_{lost} = \frac{1}{2}A_{gained}}$$

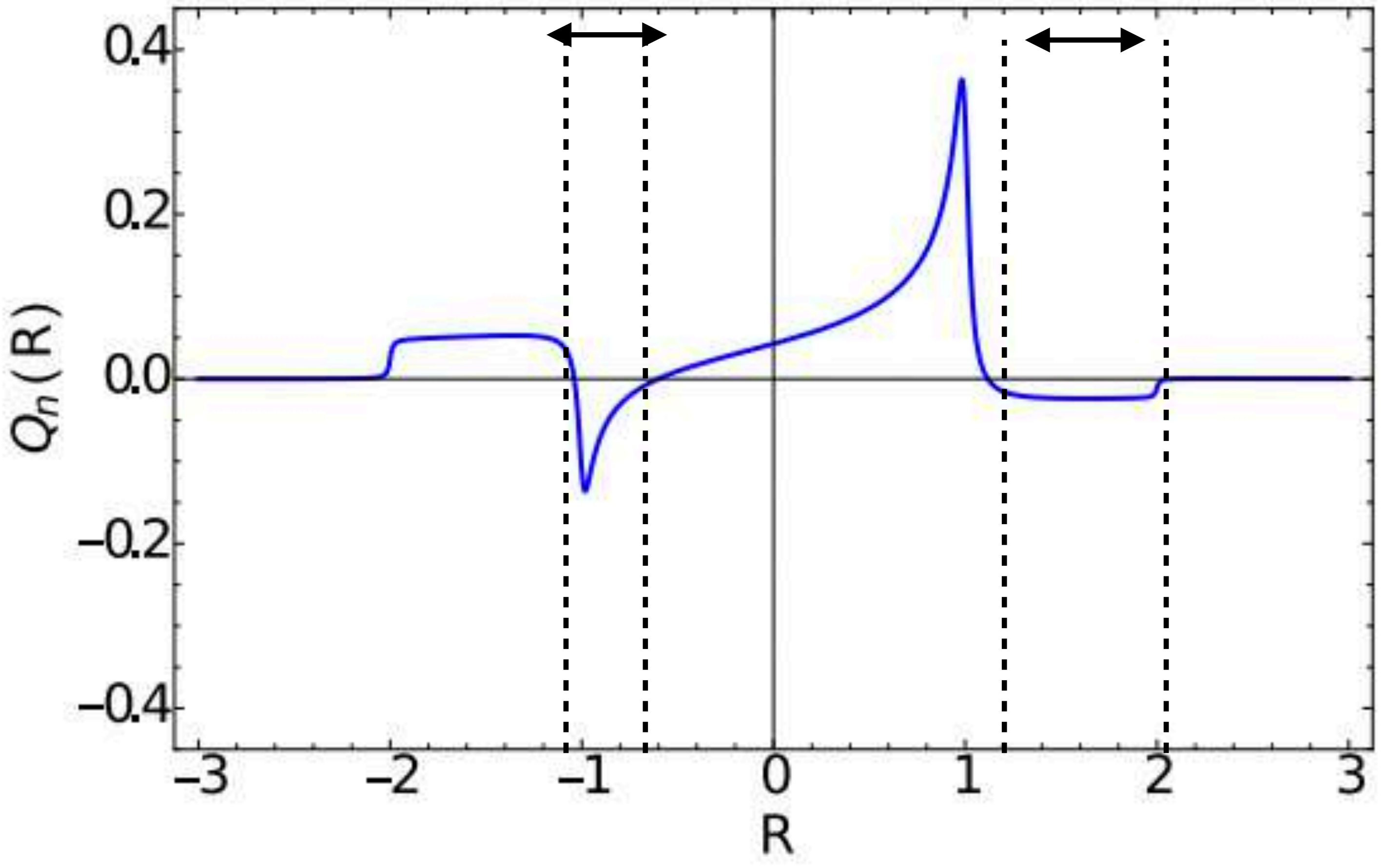
Putting These Conditions Together

Simple Measuring Tools

- The difference (Q) in intensities can by easily calculated using Boltzmann
- Apply $A_{lost} = \frac{1}{2} A_{gained}$
- Configure for any vector polarization and the particular RF region
- You're Done!!

Universally True
Any lineshape
Any material





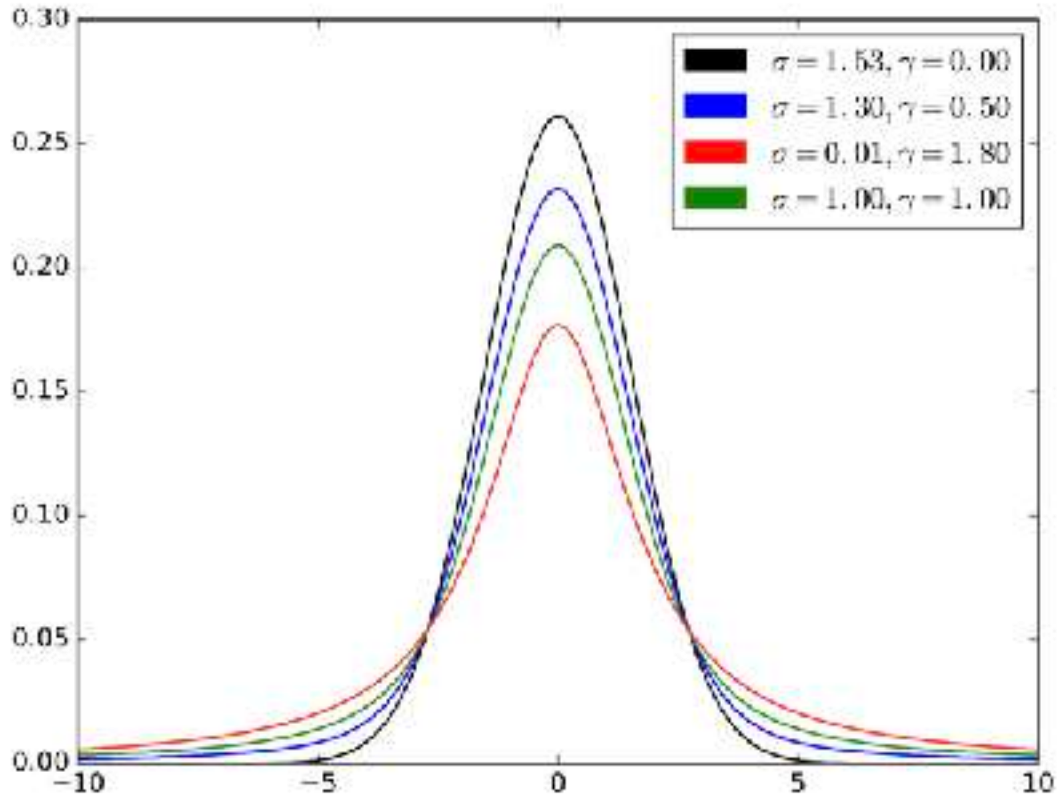
Caveats

What is exact and what is approximation

- Everything just laid out is exact for any polarization mechanism and therefor not model dependent
- Everything just laid out is in reference to longitudinal pathways and not transverse (like spin diffusion)
    - To take into account the transverse relaxation pathways one needs to fit the hole using a Voigt (convolution of Gaussian and Lorentzian)
    - These are sensitive to Q-factor of coil, degree of tuning and matching of RF circuit, amplification parameters, and transverse relaxation of material

Addressing Transverse Pathways

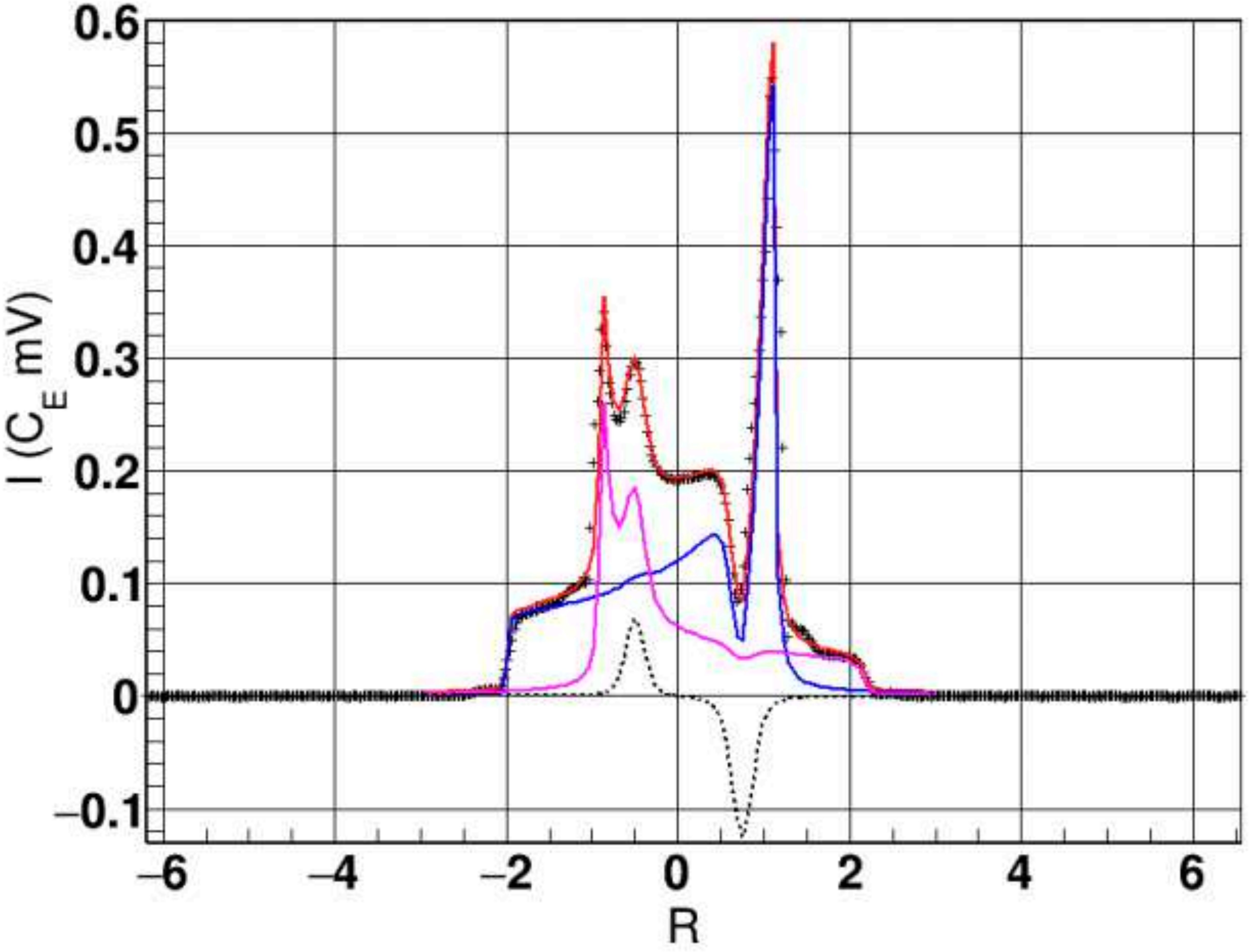
Voigt Profile



$$V(x;\sigma,\gamma) \equiv \int_{-\infty}^{\infty} G(x';\sigma) L(x-x';\gamma)\, dx'$$

$$G(x;\sigma) \equiv \frac{e^{-x^2/(2\sigma^2)}}{\sigma\sqrt{2\pi}}$$

$$L(x;\gamma) \equiv \frac{\gamma}{\pi(x^2+\gamma^2)}$$



Uncertainty Propagation

$$\left(\frac{\delta C_{TE}}{C_{TE}}\right)^2 = \left(\frac{\delta P_{TE}}{P_{TE}}\right)^2 + \left(\frac{\delta A_{TE}}{A_{TE}}\right)^2$$

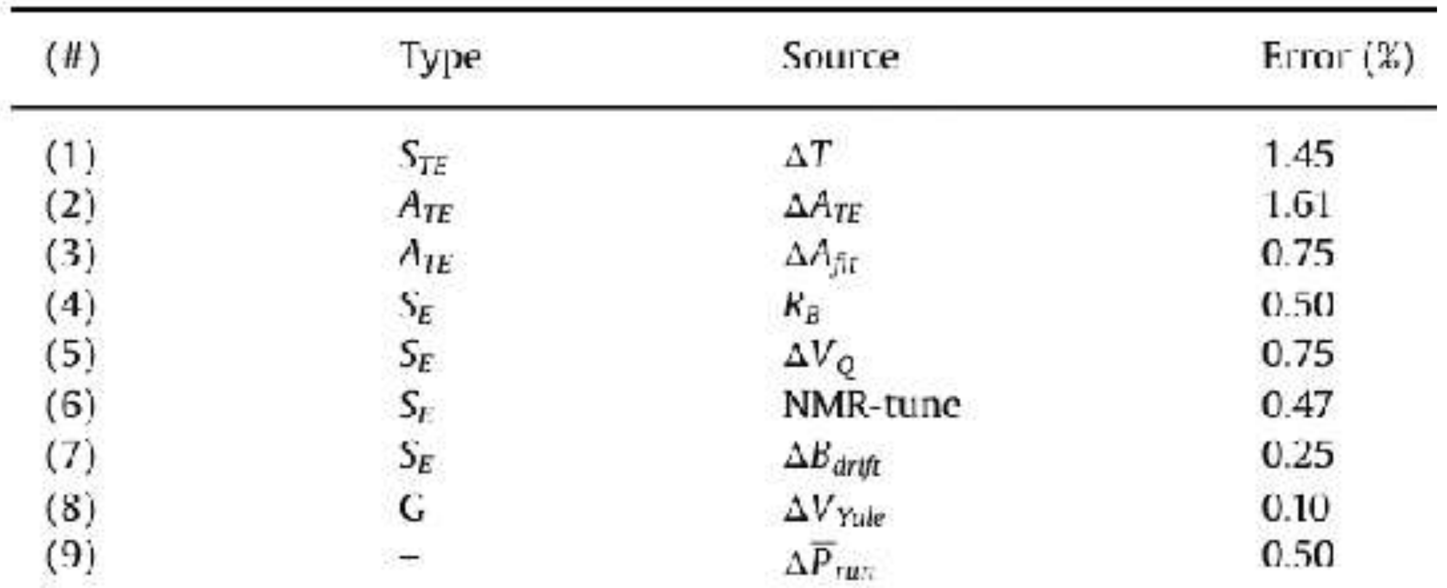
$$\frac{\delta P_E}{P_E} = \left[\left(\frac{\delta P_{TE}}{P_{TE}}\right)^2 + \left(\frac{\delta A_{TE}}{A_{TE}}\right)^2 + \left(\frac{\delta S_{TE}}{S_{TE}}\right)^2 + \left(\frac{\delta A_E}{A_E}\right)^2 + \left(\frac{\delta S_E}{S_E}\right)^2 + \left(\frac{\delta G}{G}\right)^2\right]^{1/2}$$

① A_{TE} - Relative uncertainties in area acquired during TE

② S_{TE} - Measurement limitation during TE

③ S_E - Systematic variation in enhanced signal

④ G - Error from gain



(#)	Type	Source	Error (%)
(1)	S_{TE}	ΔT	1.45
(2)	A_{TE}	ΔA_{TE}	1.61
(3)	A_{TE}	ΔA_{fit}	0.75
(4)	S_E	R_B	0.50
(5)	S_E	ΔV_Q	0.75
(6)	S_E	NMR-tune	0.47
(7)	S_E	ΔB_{drift}	0.25
(8)	G	ΔV_{Yule}	0.10
(9)	–	$\Delta \overline{P}_{run}$	0.50

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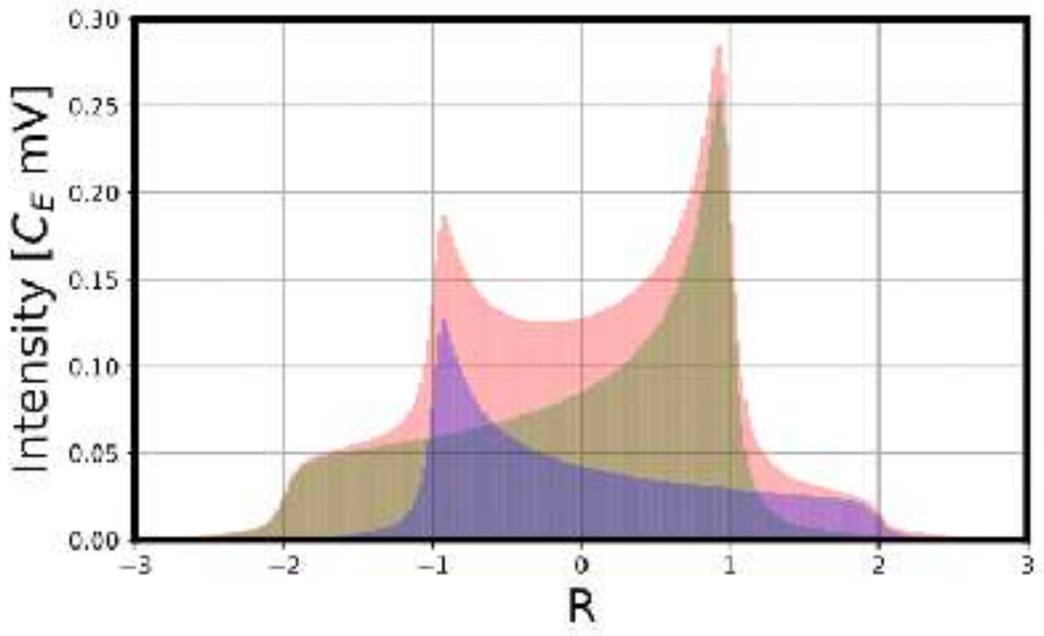
Additional Contributions (Steady-State)

$$\delta I_{\pm} = \sqrt{(\delta C)^2 + (\delta A_{\chi^2})^2 + (\delta A_{\partial t})}$$

- (δC) Standard Contributions from above
- (δA_{χ^2}) Variation in area over covariance matrix minimization
- $(\delta A_{\partial t})$ NMR measurement limitations with respects to relaxation rate

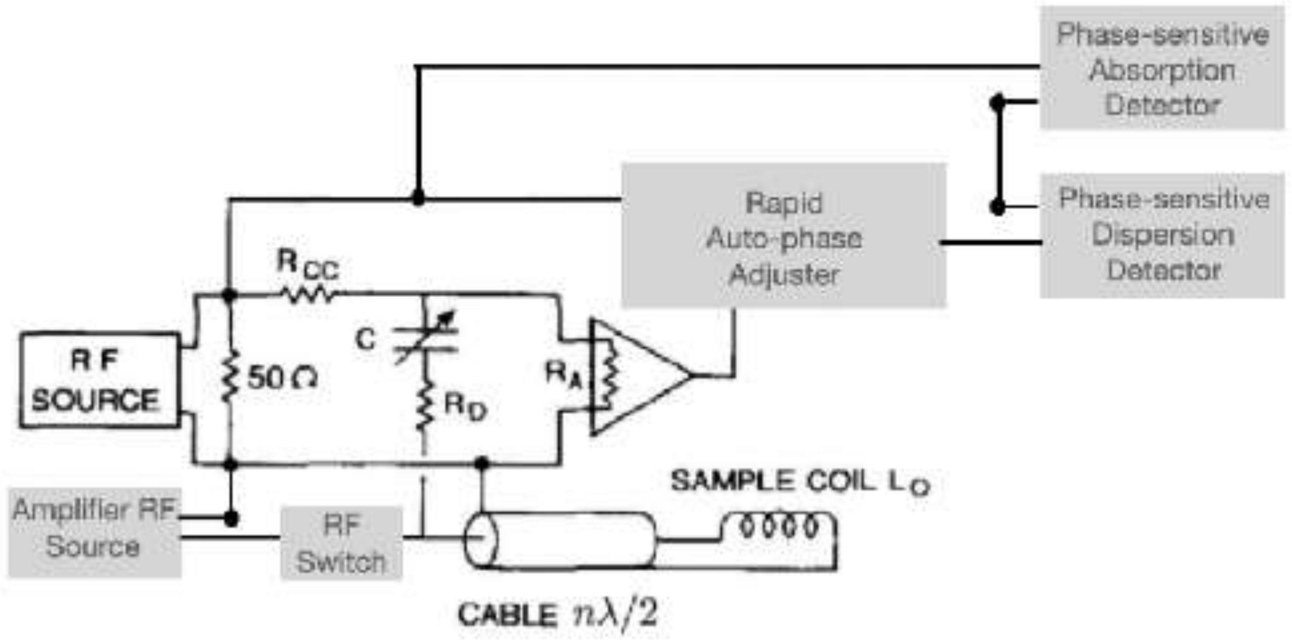
Modern Uncertainty Measurement

- Produce a simulated signal
- Extract using modern measurement tools
- Mininize deviation



Modern Measurement Tools

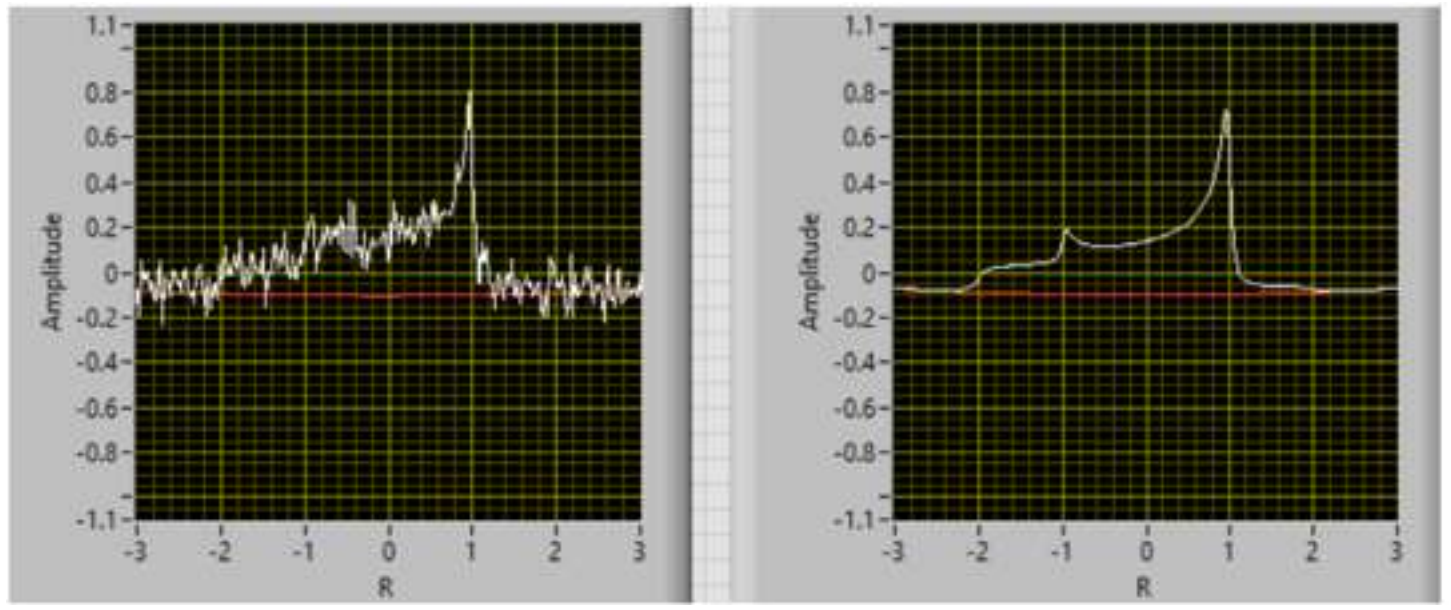
Specialized for application

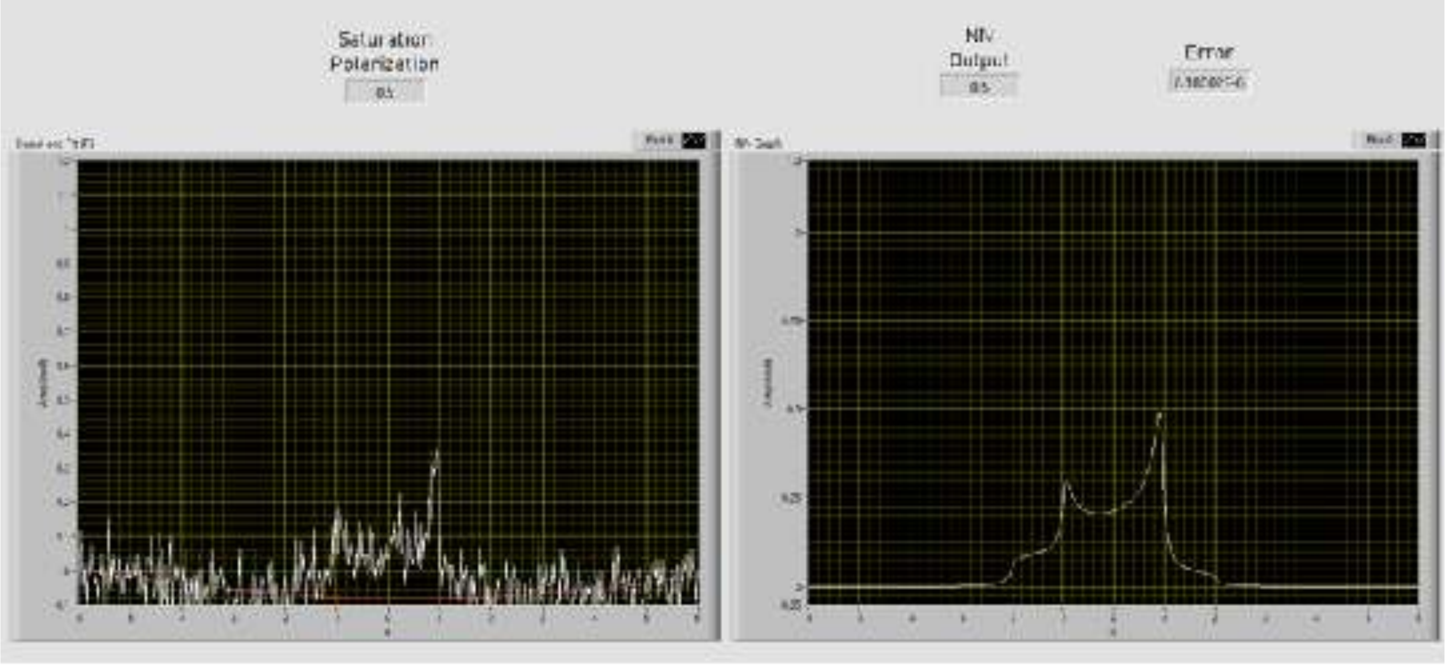


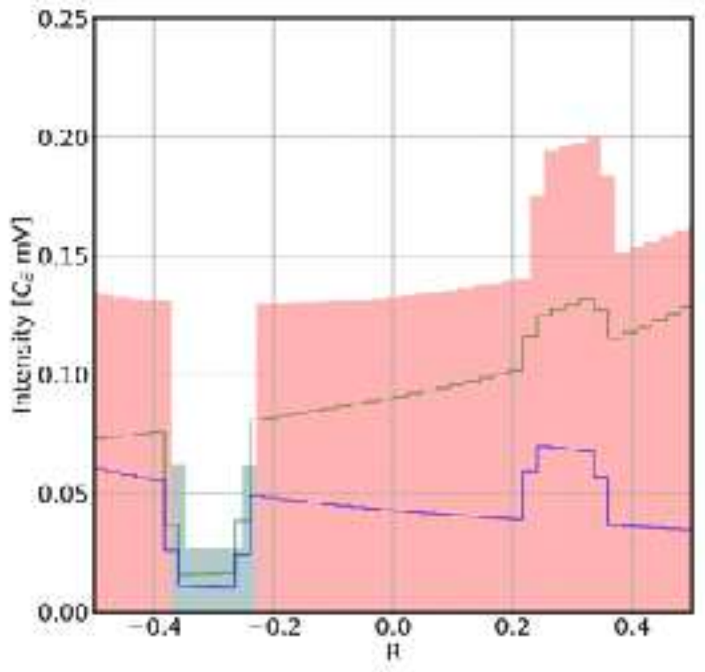
With this design, the reference signal is supplied to the mixer while being modulated rapidly (~MHz) using a programmable auto-phase adjuster, from a dedicated phase shifter. The reference is then broken into the real and imaginary parts of the signal and passed to the analyzer which uses fast signal integration to produce 1000 phase-shifted measurements and a CW dispersion measurement simultaneously. This information is then sent to the RF controls to make the polarization measurements and adjust the RF modulation across the frequency domain to continuously tune and optimize the signal.

UVA has prototyped this type of system and is presently studying the required design parameters and determining how best to fully integrate this new system into modered DAQ and monitoring electronics. We are also looking into how to attract funds to build this system.

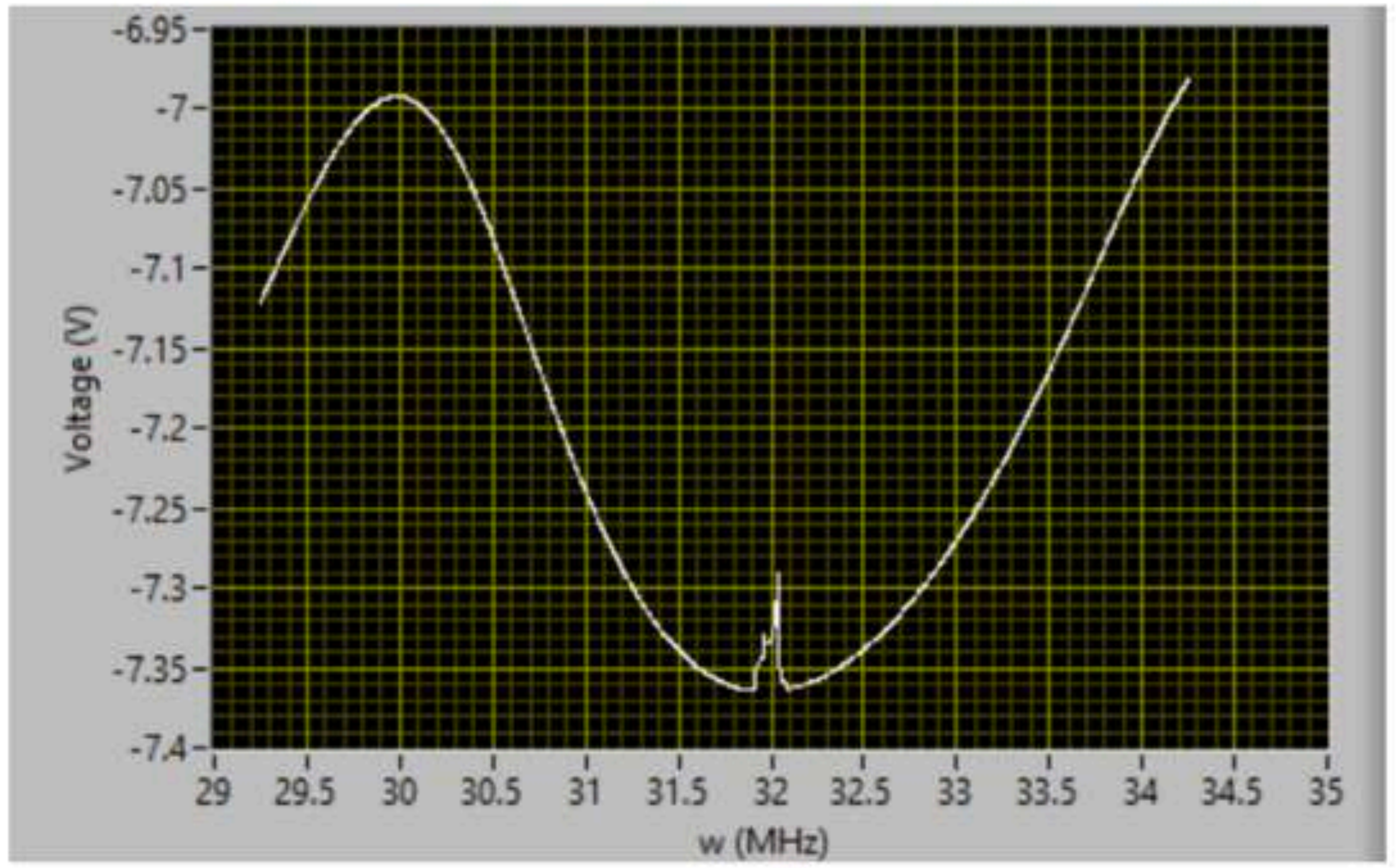
Instrumentation Advancement

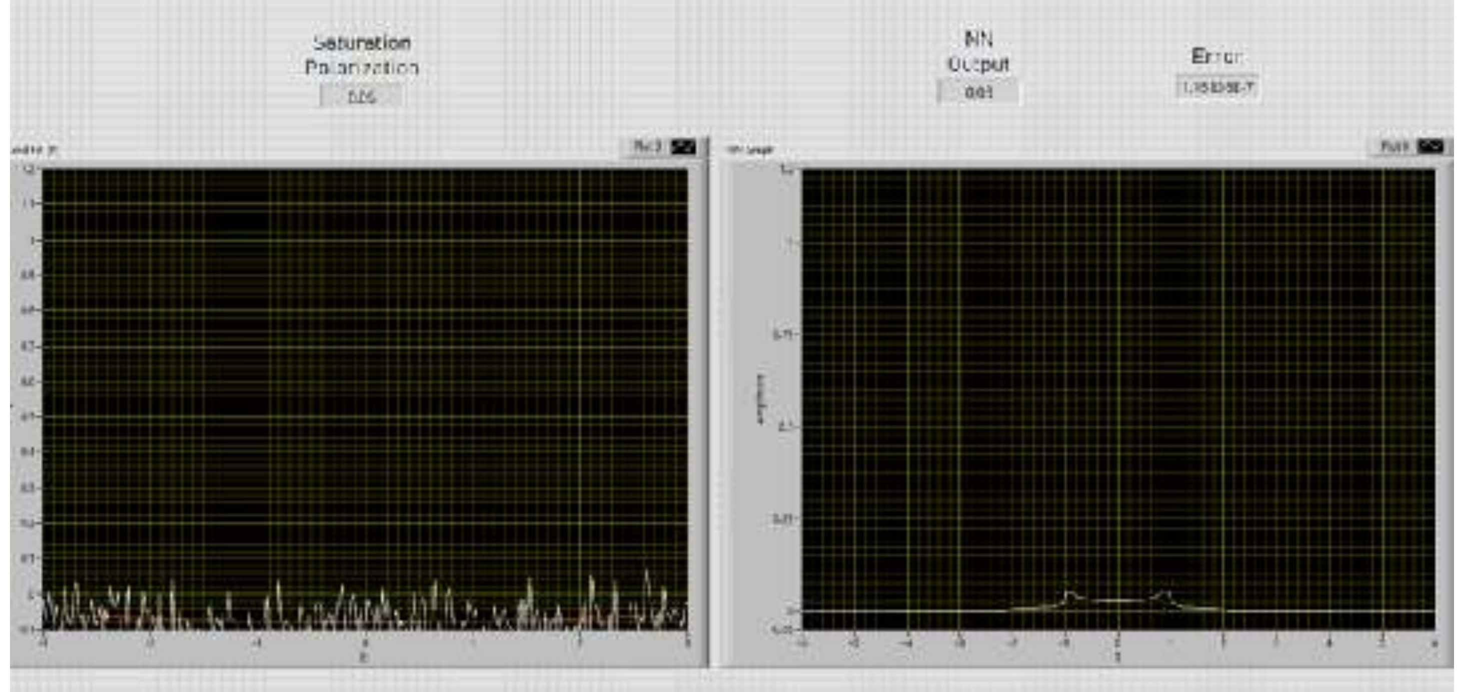




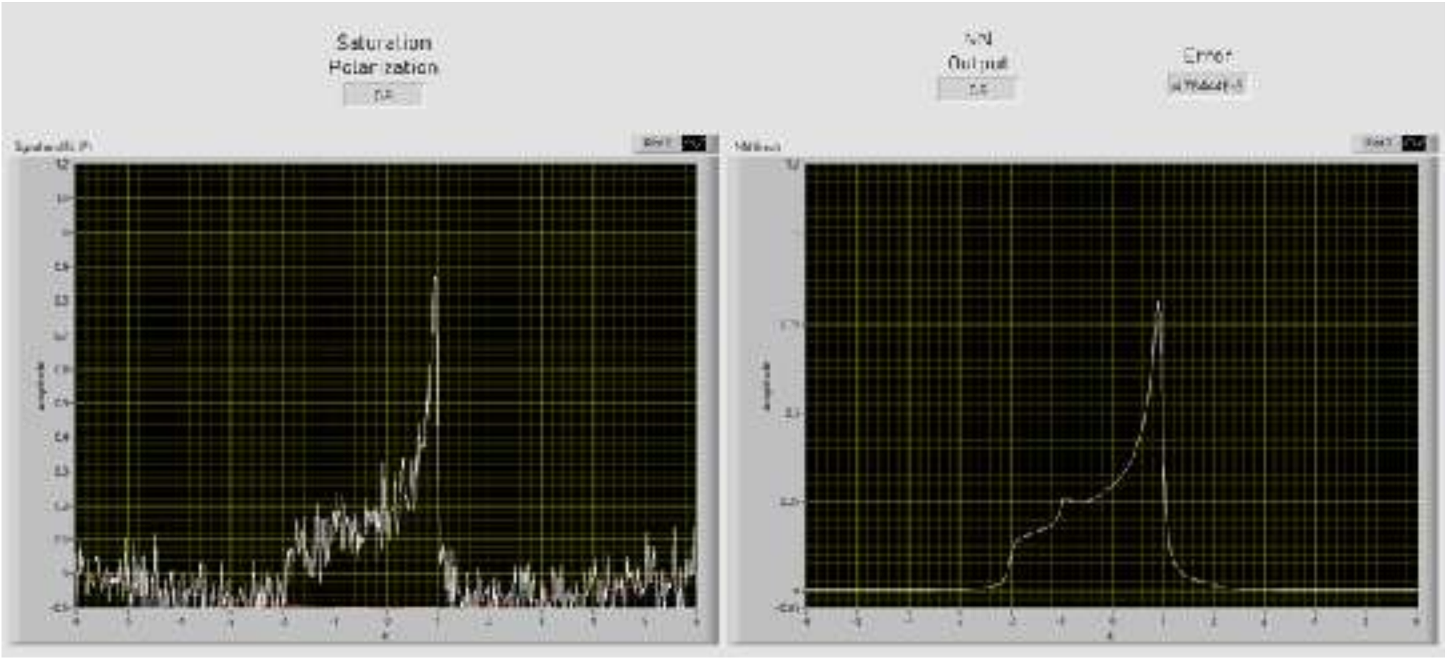


Q-Meter Simulation





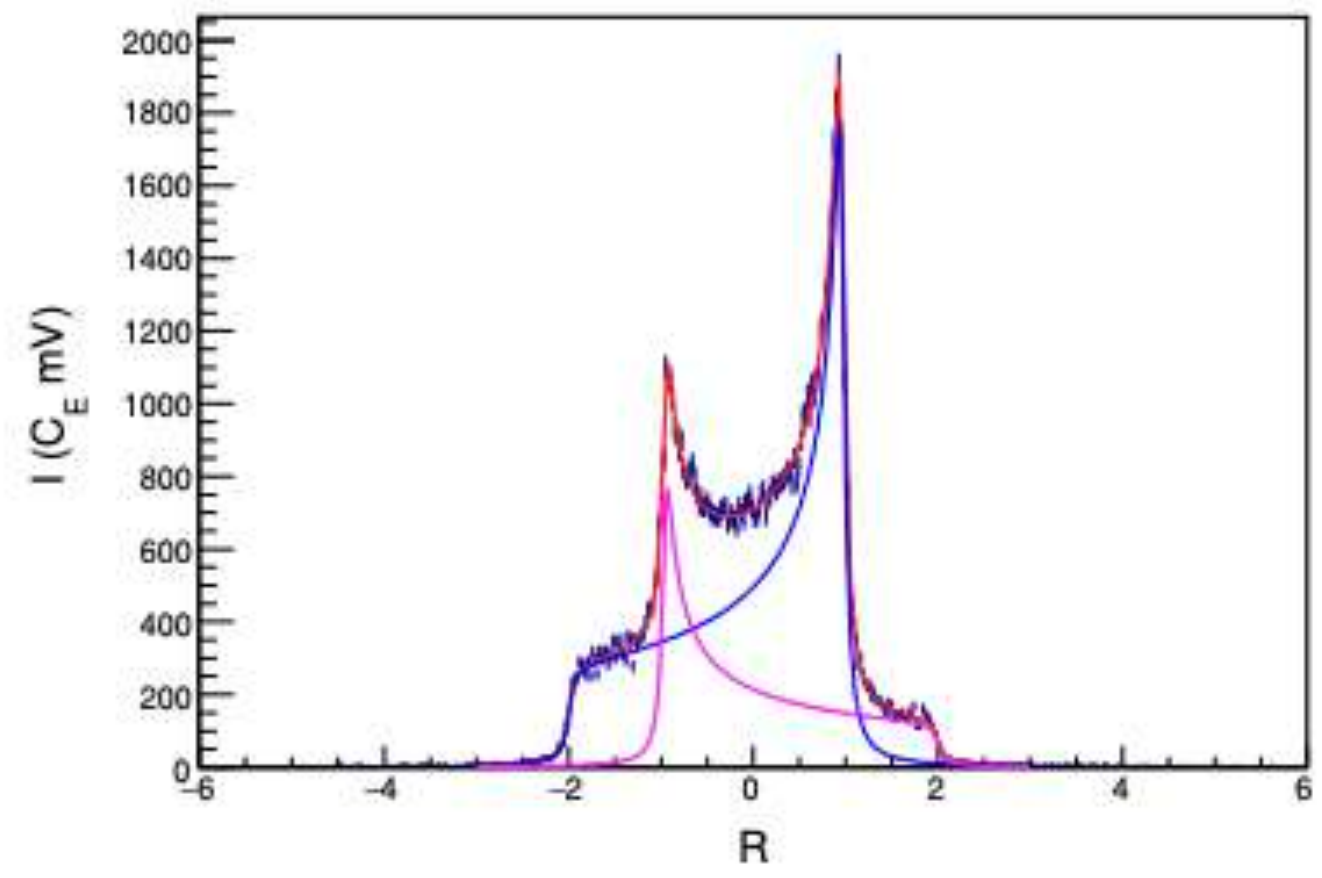
ANN with NMR

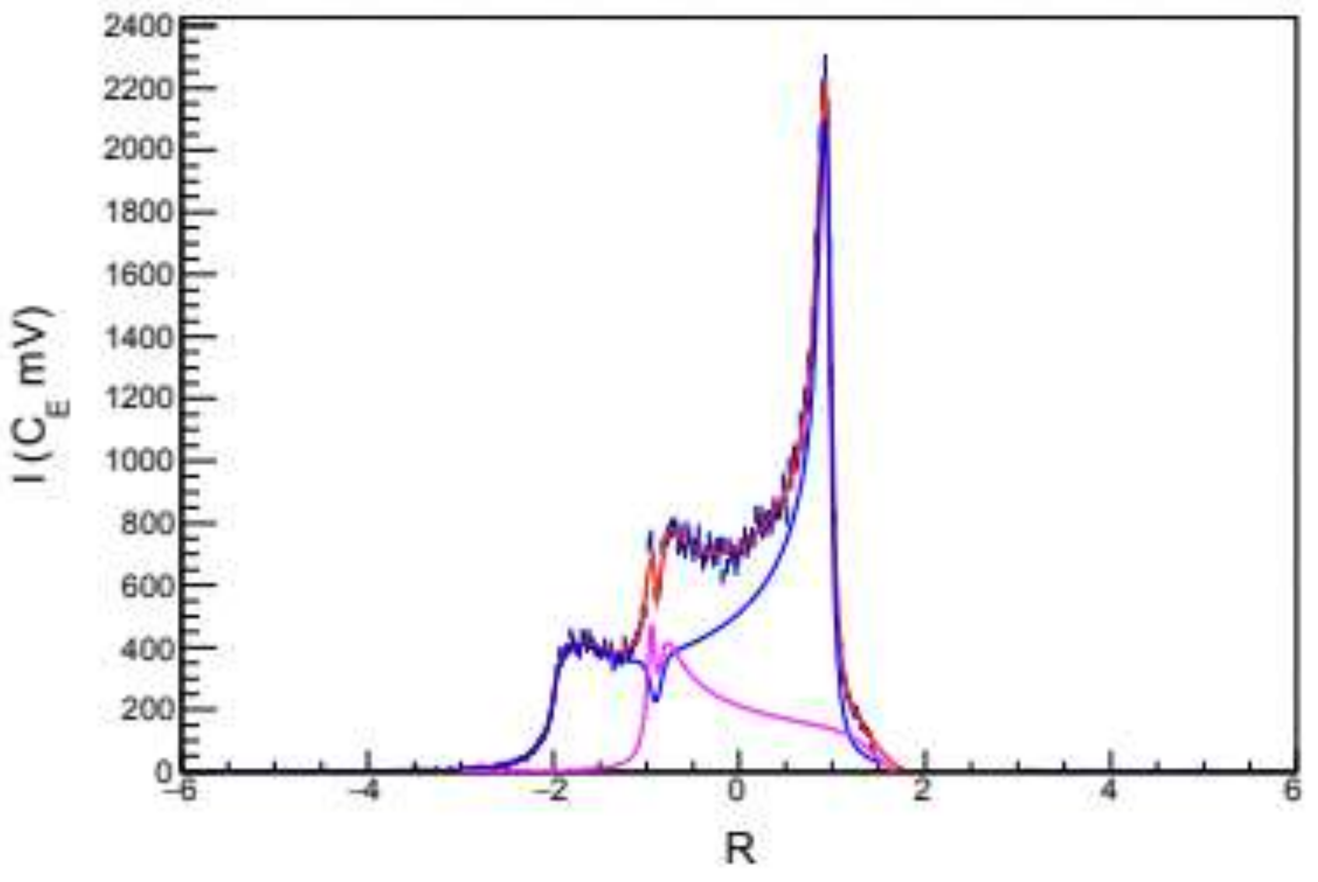


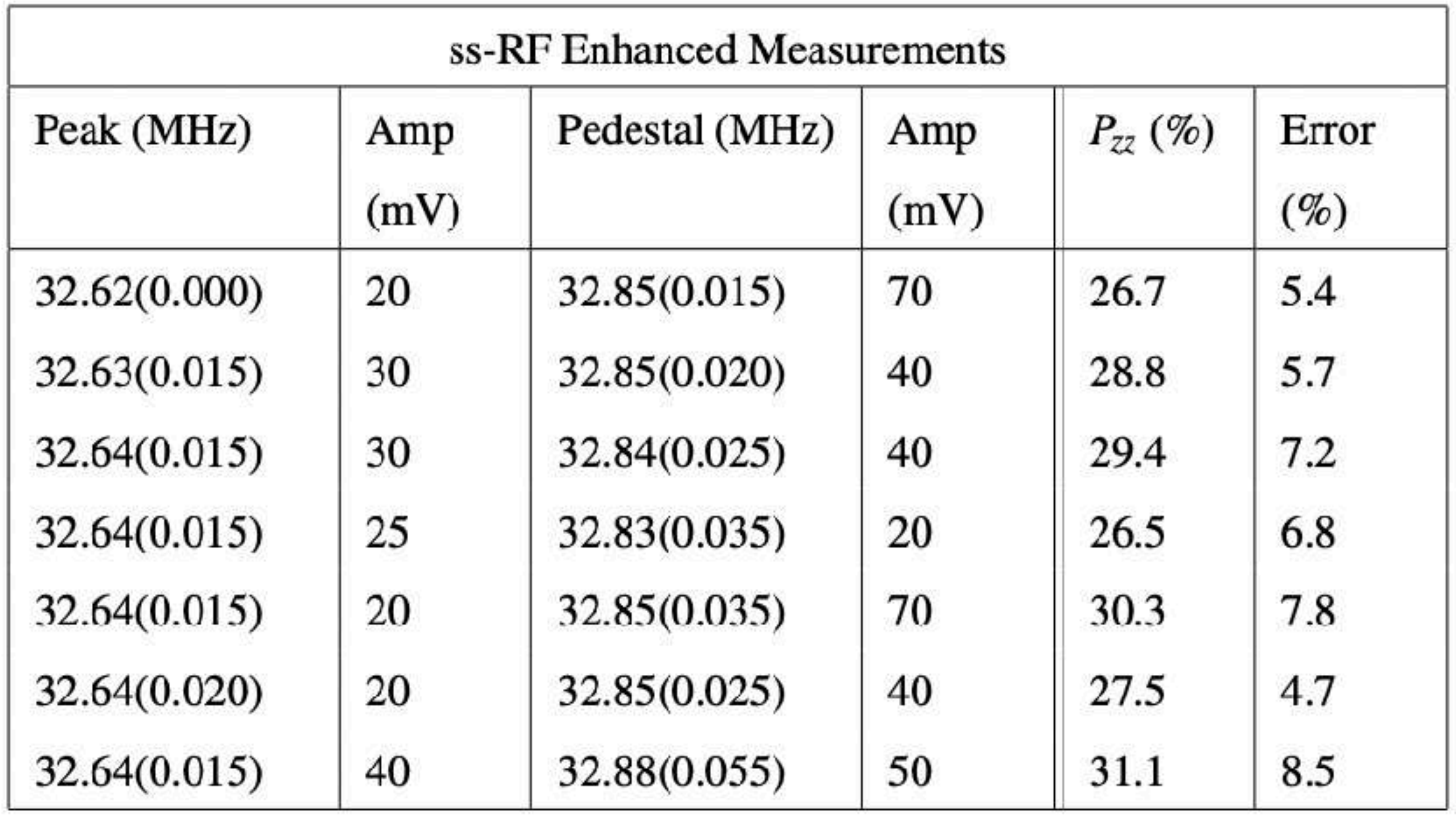
Software Advancement

Measurements of Tensor Enhancement

Experimental results (all with irradiated d-Butanol)







ss-RF Enhanced Measurements					
Peak (MHz)	Amp (mV)	Pedestal (MHz)	Amp (mV)	P_{zz} (%)	Error (%)
32.62(0.000)	20	32.85(0.015)	70	26.7	5.4
32.63(0.015)	30	32.85(0.020)	40	28.8	5.7
32.64(0.015)	30	32.84(0.025)	40	29.4	7.2
32.64(0.015)	25	32.83(0.035)	20	26.5	6.8
32.64(0.015)	20	32.85(0.035)	70	30.3	7.8
32.64(0.020)	20	32.85(0.025)	40	27.5	4.7
32.64(0.015)	40	32.88(0.055)	50	31.1	8.5

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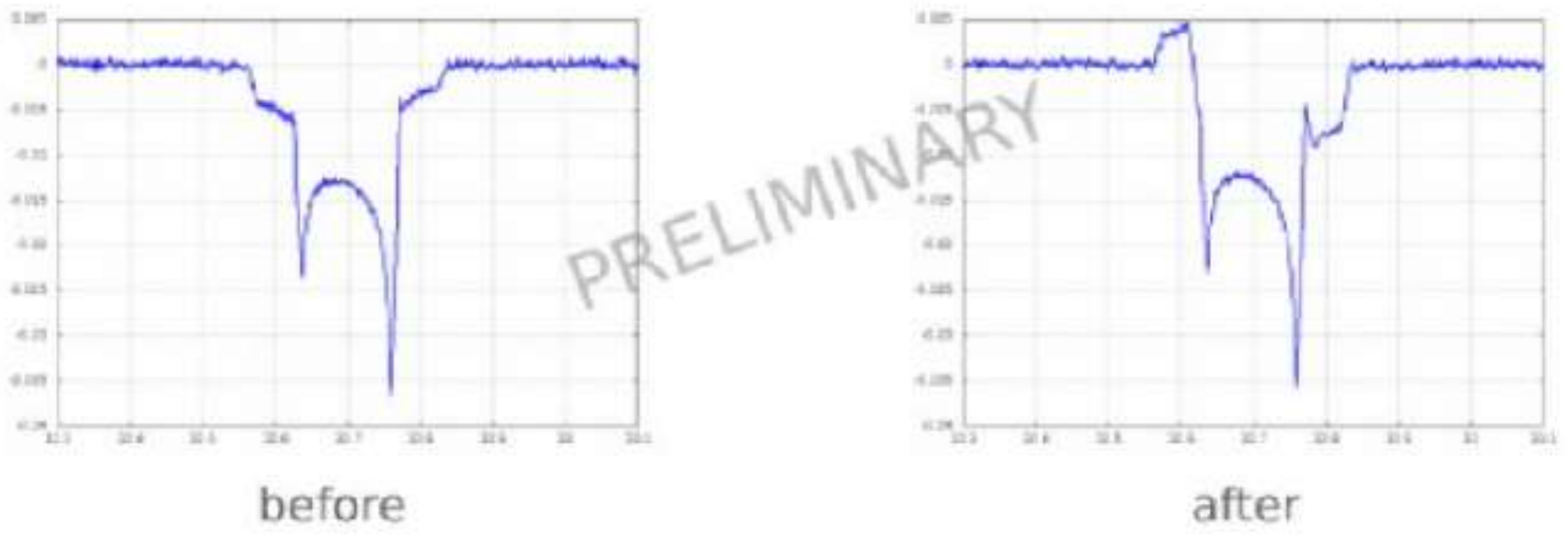
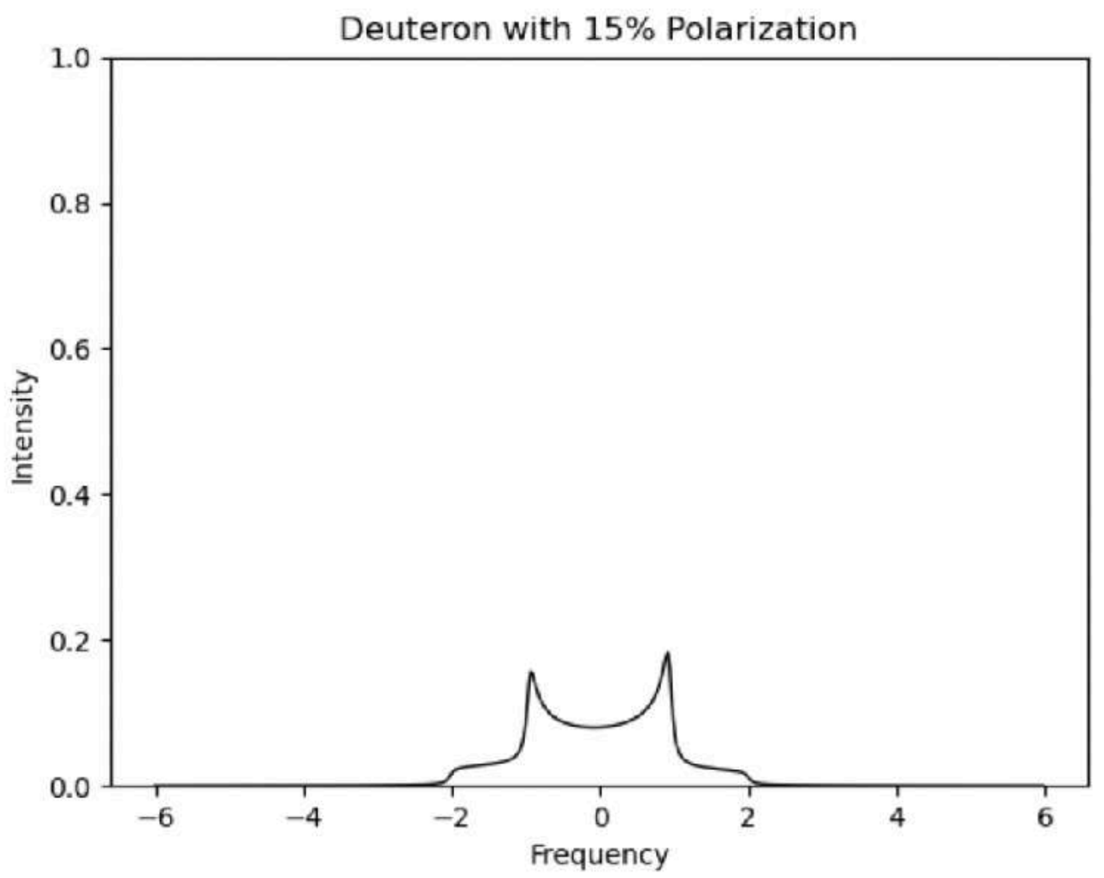
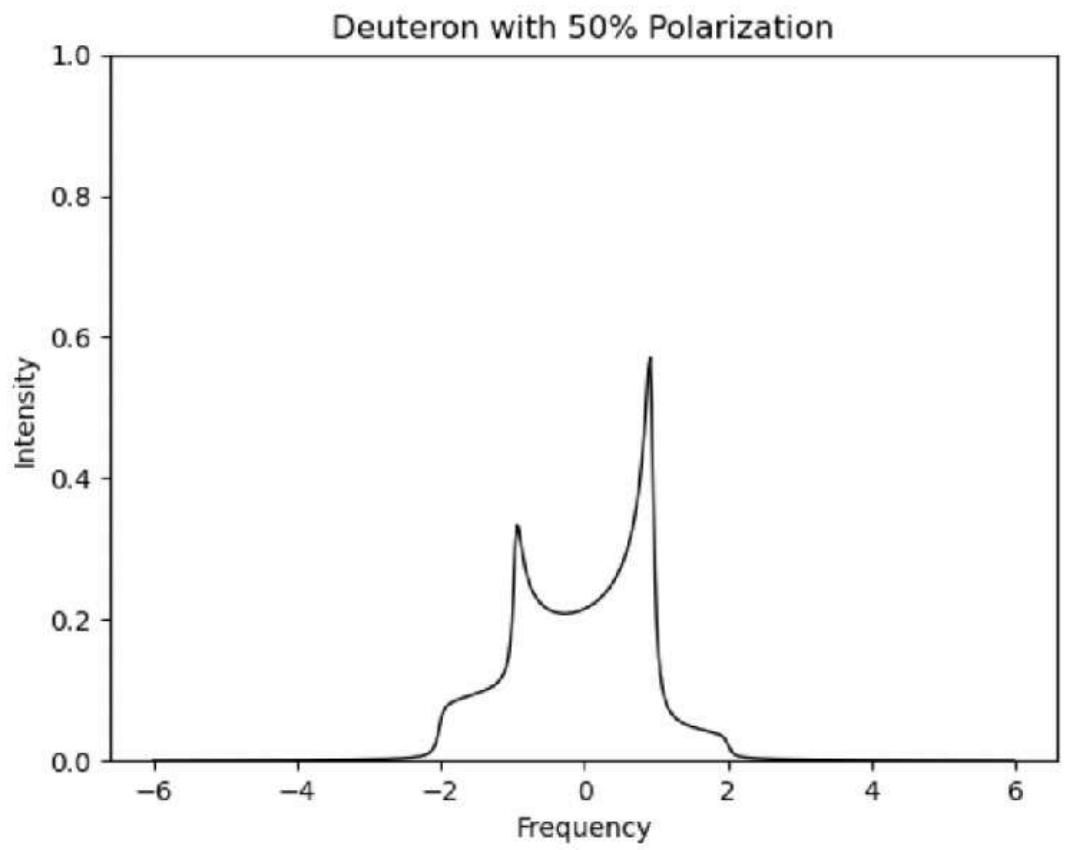
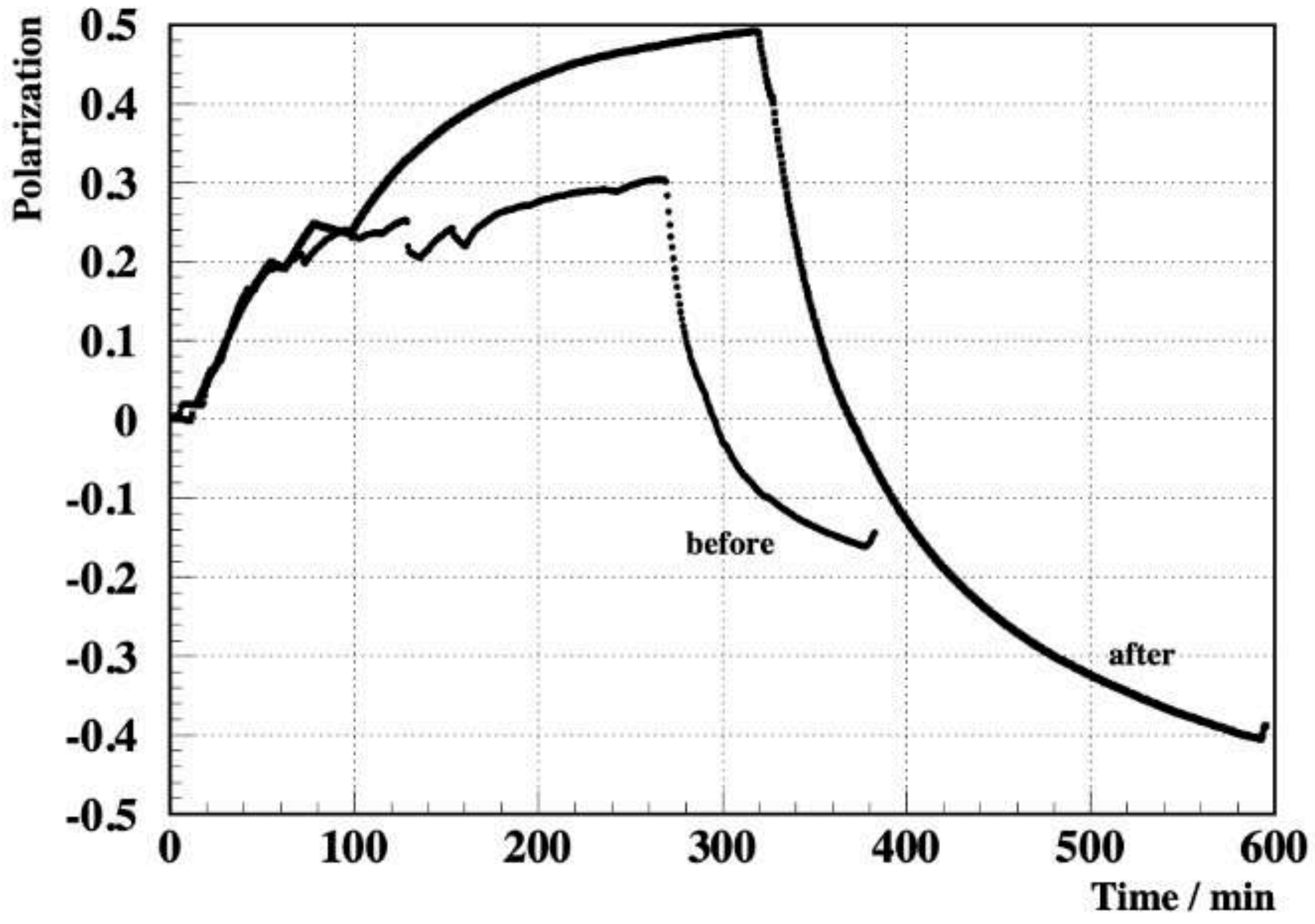


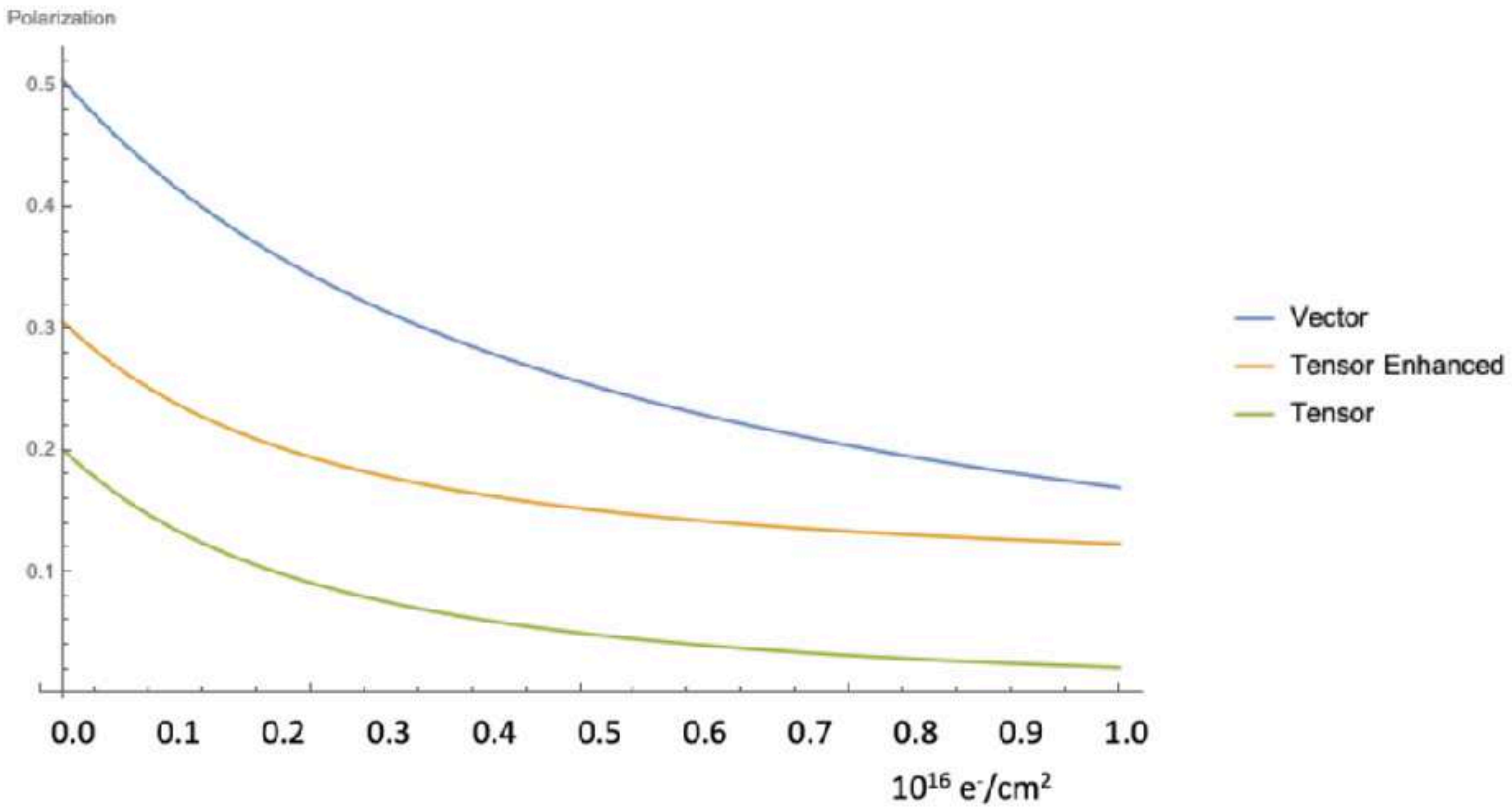
Charge-3

Change as a Function of Dose





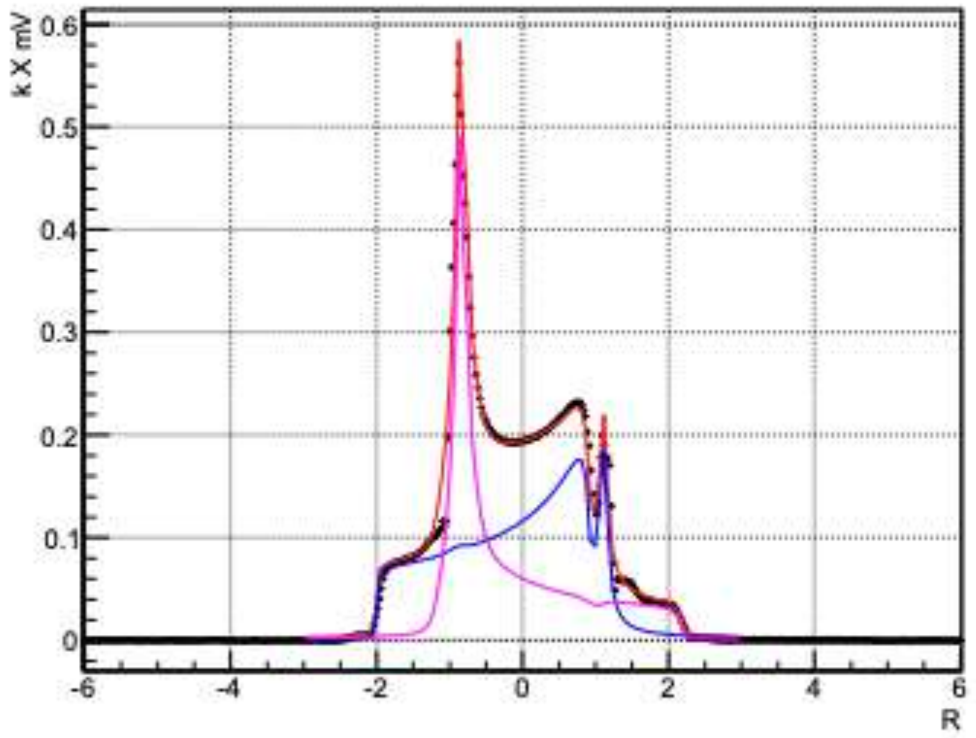




Charge-4

The Experimental Situation and Rotation

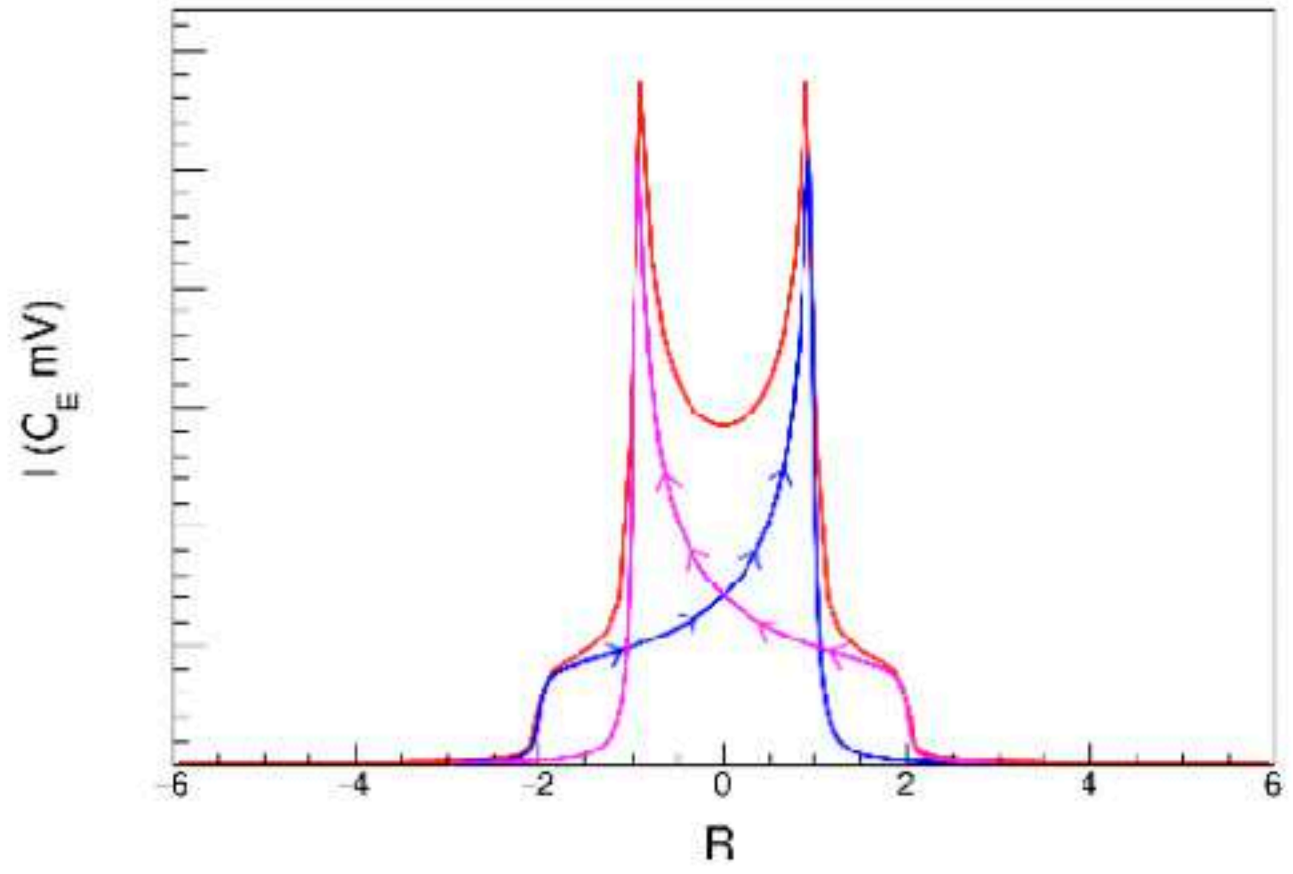
- ss-RF can be used to enhance the tensor polarization (average) over the course of the experiment even as vector polarization decays
- Modern measurement tools can be implemented to a relative error ~2%
- It benefits us to use (+/-)vector polarized target with zero tensor alternating with a tensor enhanced state, this can be done quick (~secs)
- Other enhancement tools still under development

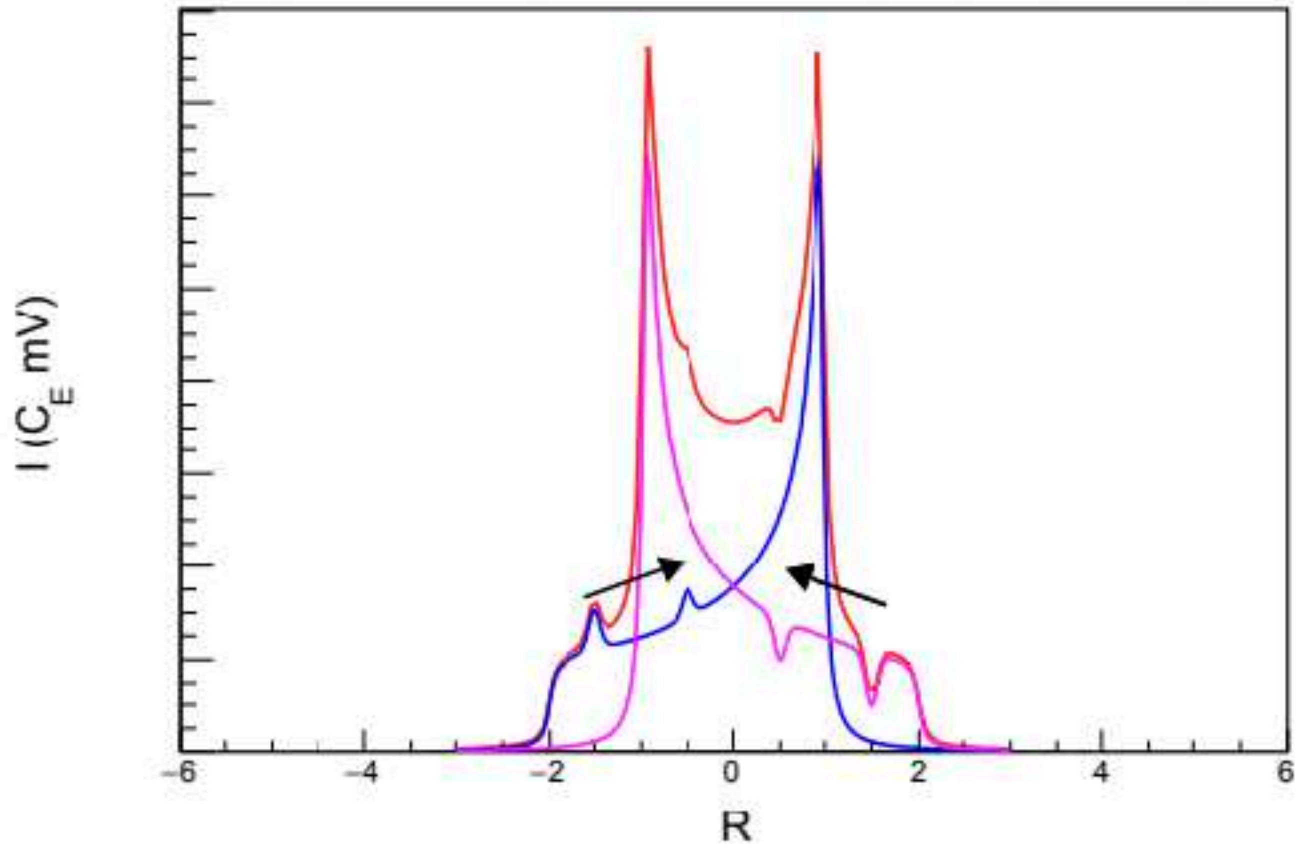


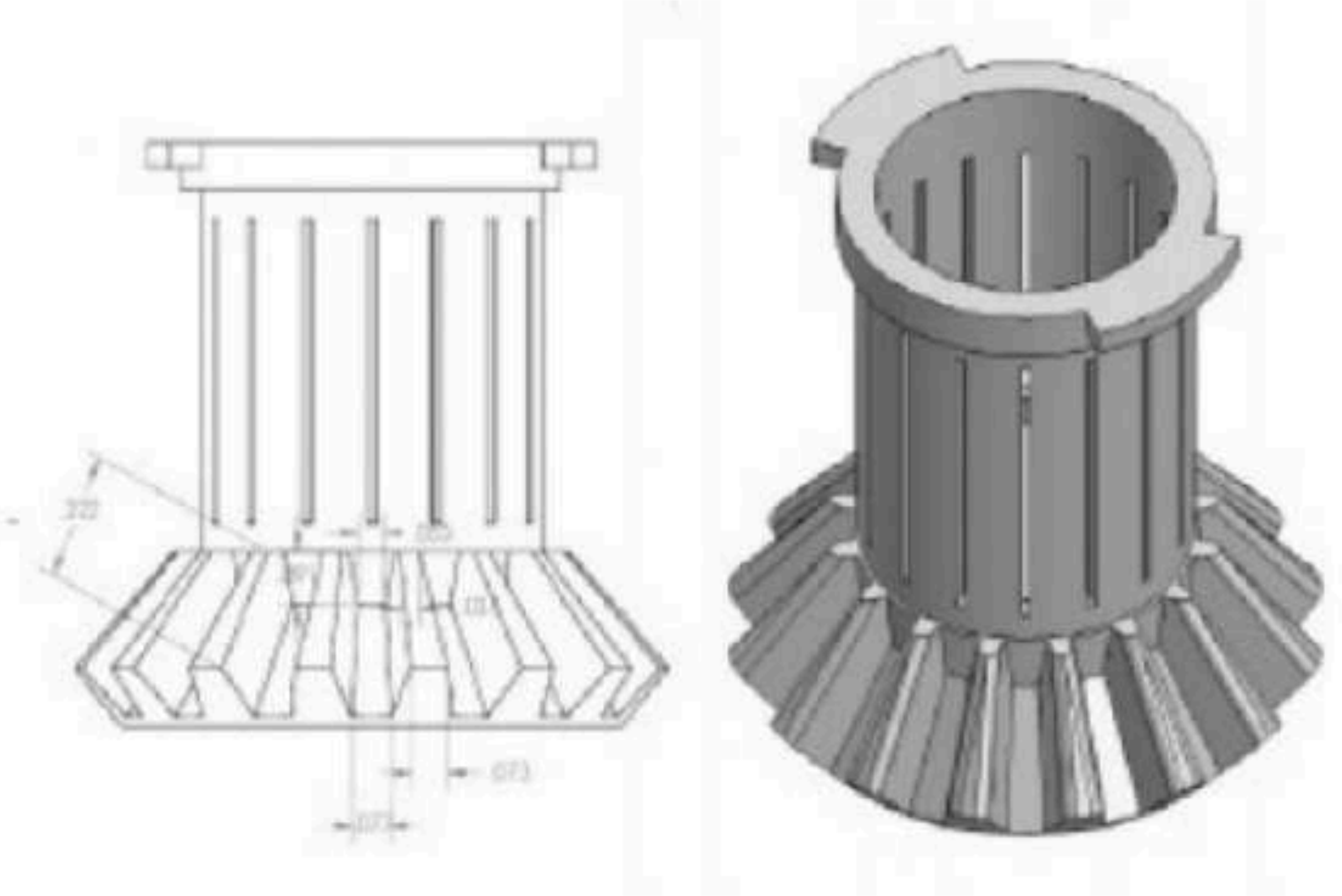
Rotating Targets (work still in progress)

And results (slow rotation)

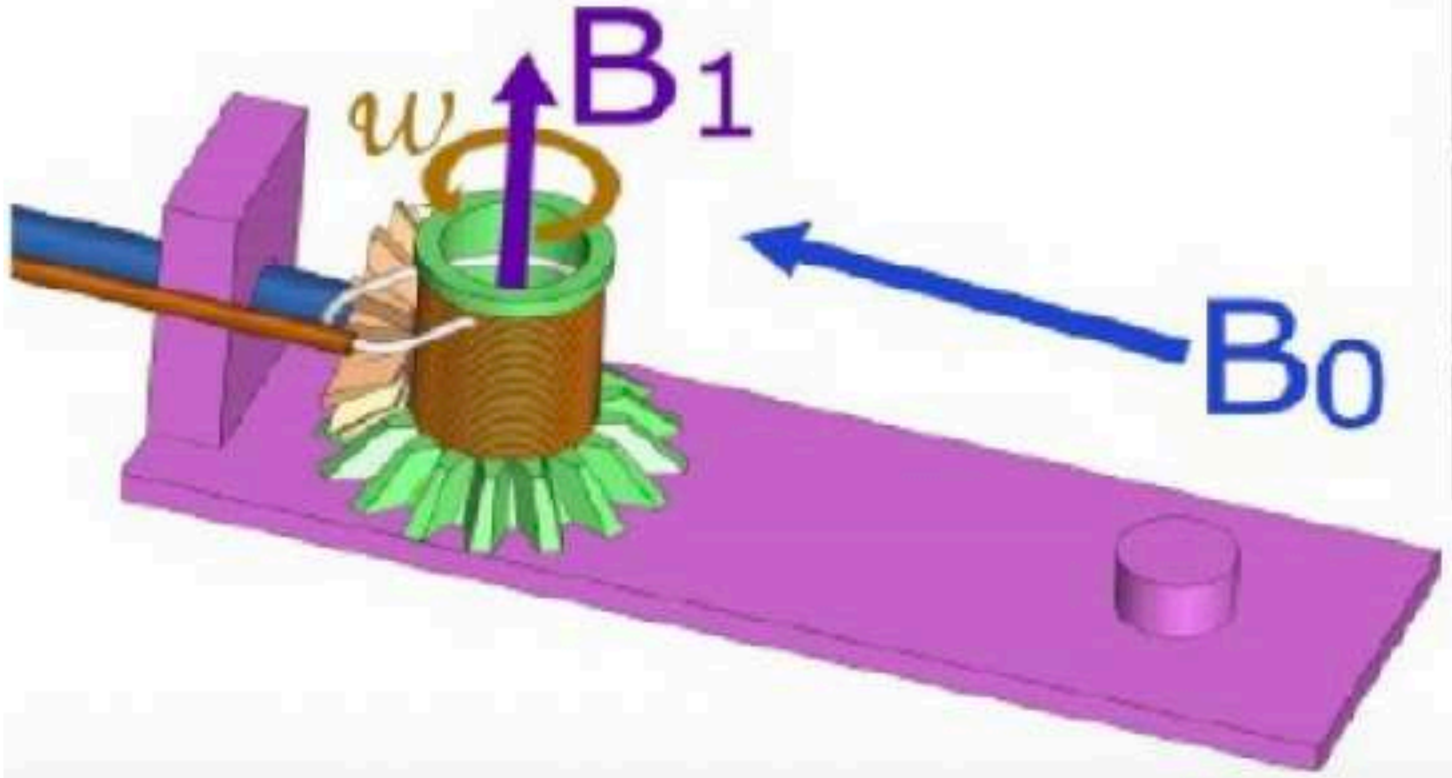
- Rotate to TRY to burn one entire absorption line
- Spin Diffusion fights repopulates with rotation but changes for every angle

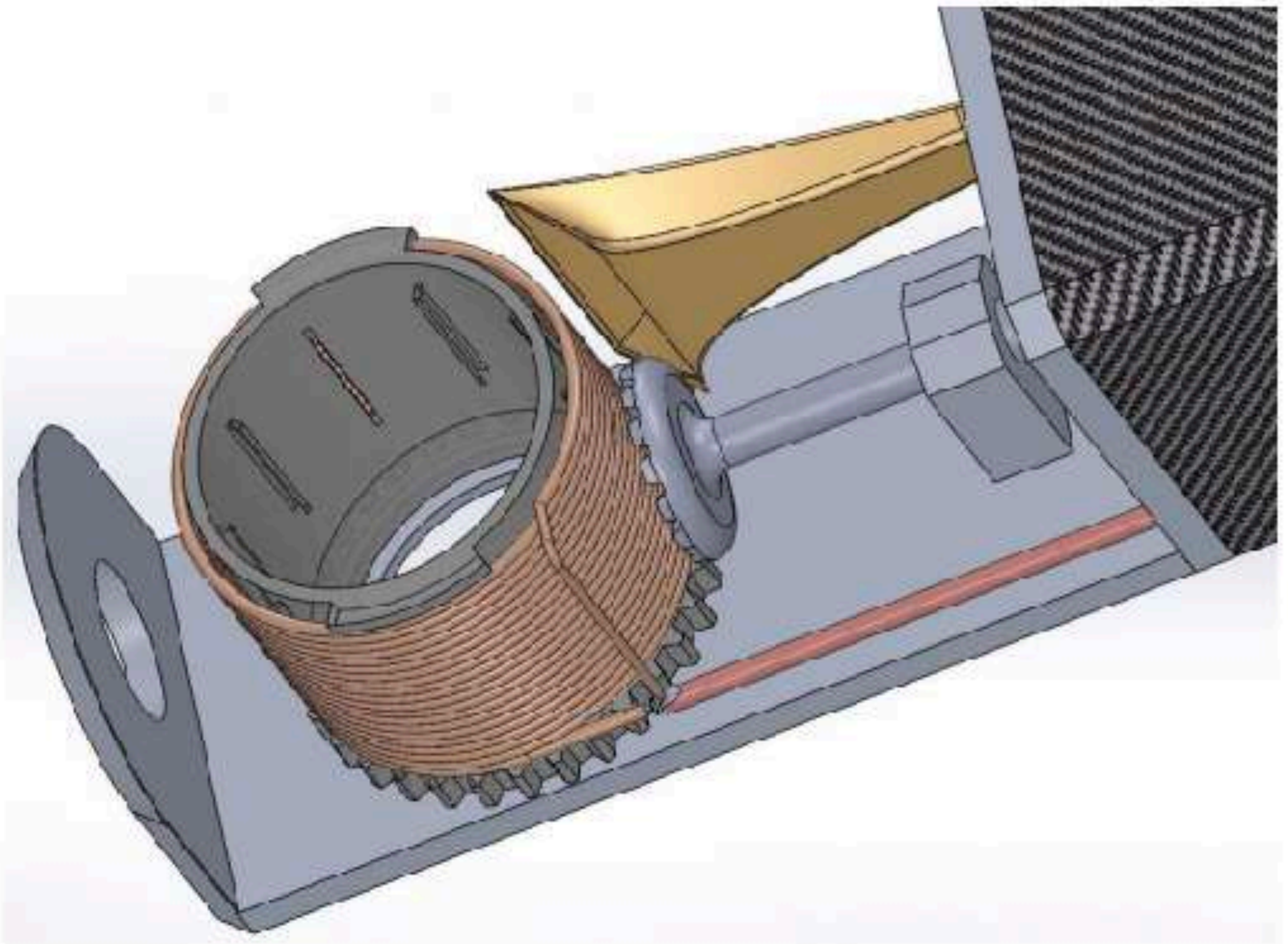


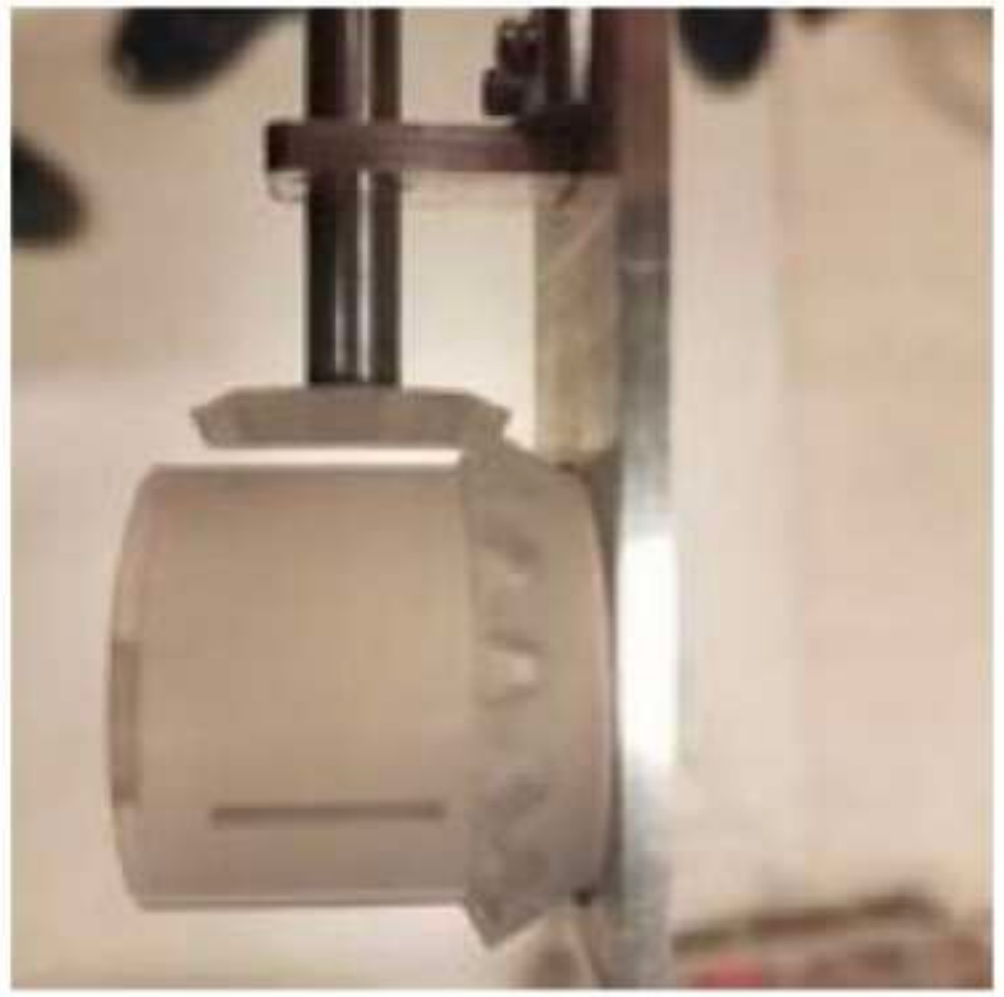




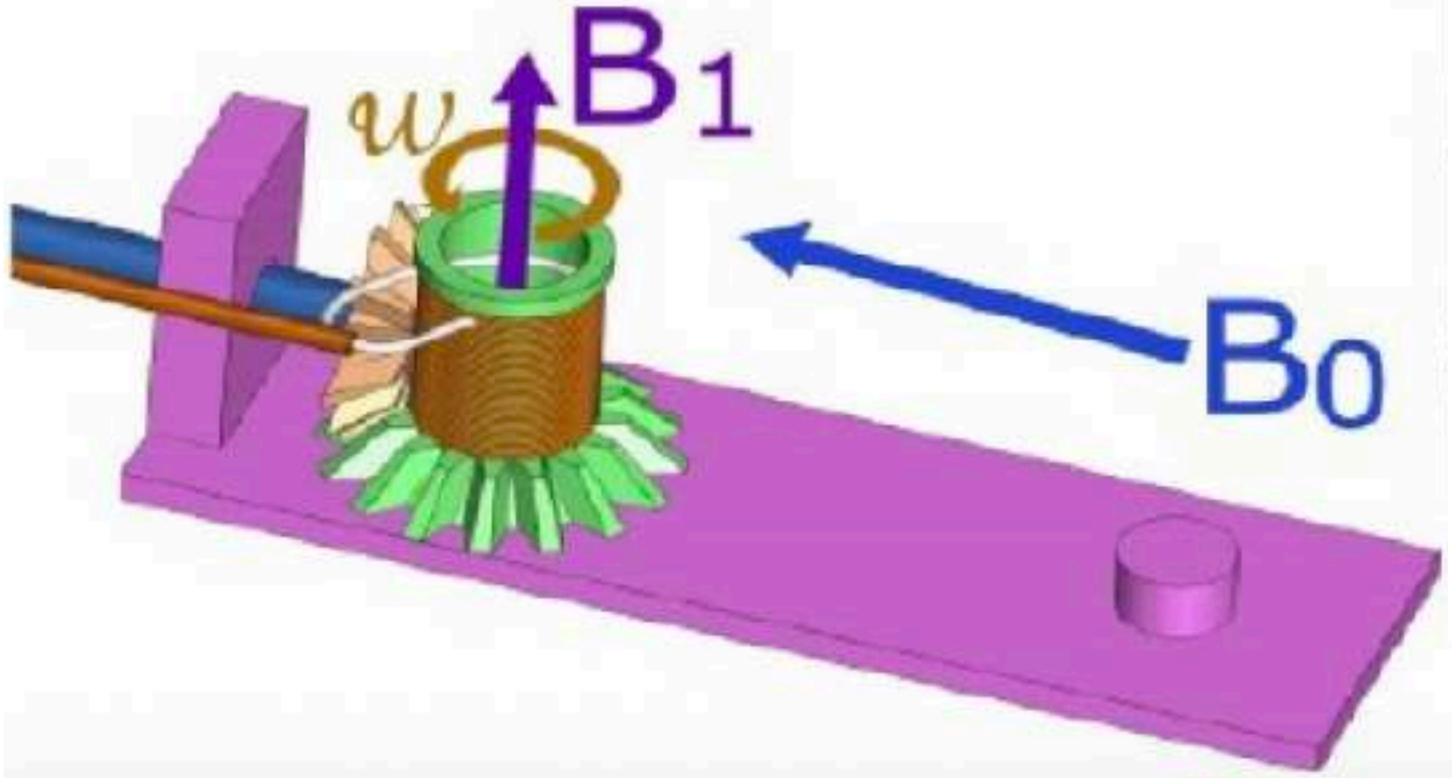
- Kel-F $(C_2ClF_3)_n$ cup and driving gear
- Motor outside cryostat
- NMR coil around cup
- Already used with several designs at UVA
- 1 Hz achieved with no problem
- Fixed beam spot

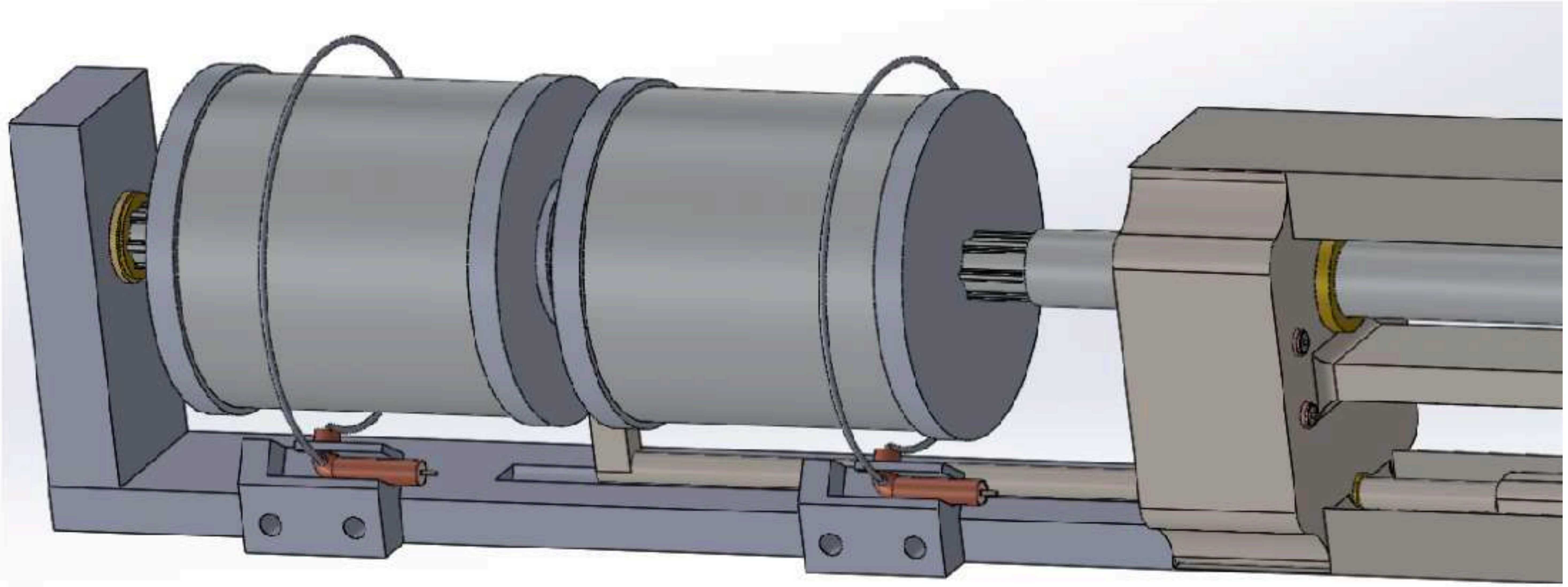






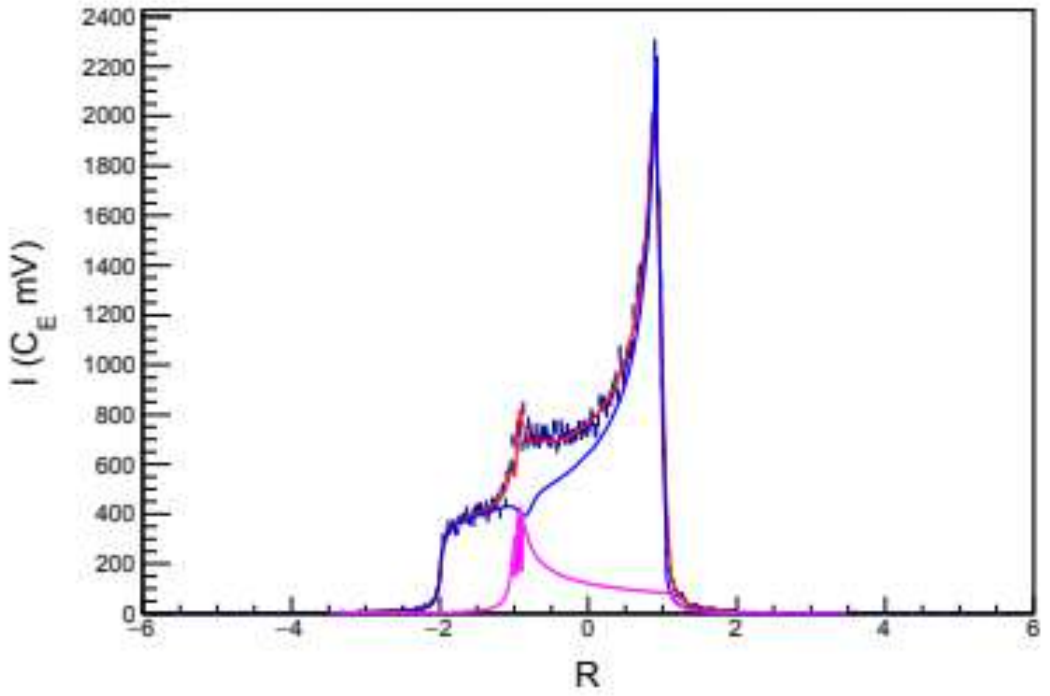
- Motor outside cryostat
- NMR coil around cup
- Already used with several designs at UVA
- 1 Hz achieved with no problem
- Fixed beam spot



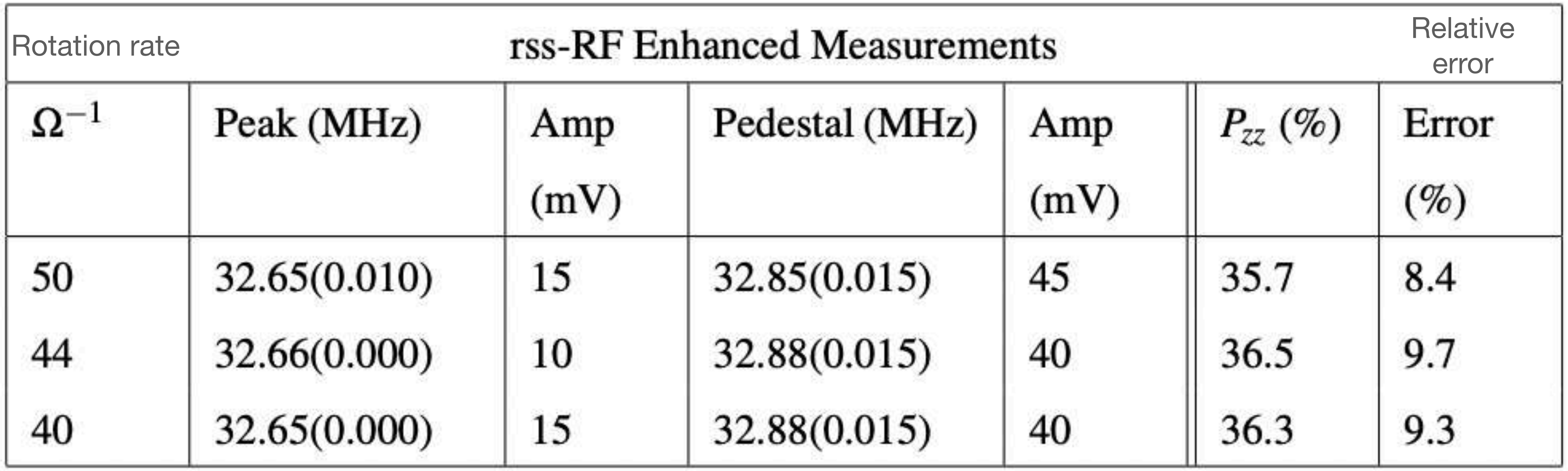


Rotation Results

10% relative uncertainty is the best we can do with rotation



At <40° with respects to B



Rotation rate	rss-RF Enhanced Measurements					Relative error
Ω^{-1}	Peak (MHz)	Amp (mV)	Pedestal (MHz)	Amp (mV)	P_{zz} (%)	Error (%)
50	32.65(0.010)	15	32.85(0.015)	45	35.7	8.4
44	32.66(0.000)	10	32.88(0.015)	40	36.5	9.7
40	32.65(0.000)	15	32.88(0.015)	40	36.3	9.3

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Conclusion

- We have the tools to be able to run the b1 and Azz experiments today and get a good measurement
- We need full approval to ramp up our development effort and attract the funds to be able to build modern instrumentation that will allow us to take full advantage of our new technology
- We will continue in the research and development of tensor polarization enhancement and expect to continue to improve