Polarization Optimization and Measurement for Solid Spin-1 Targets

for the 22nd International Spin Symposium

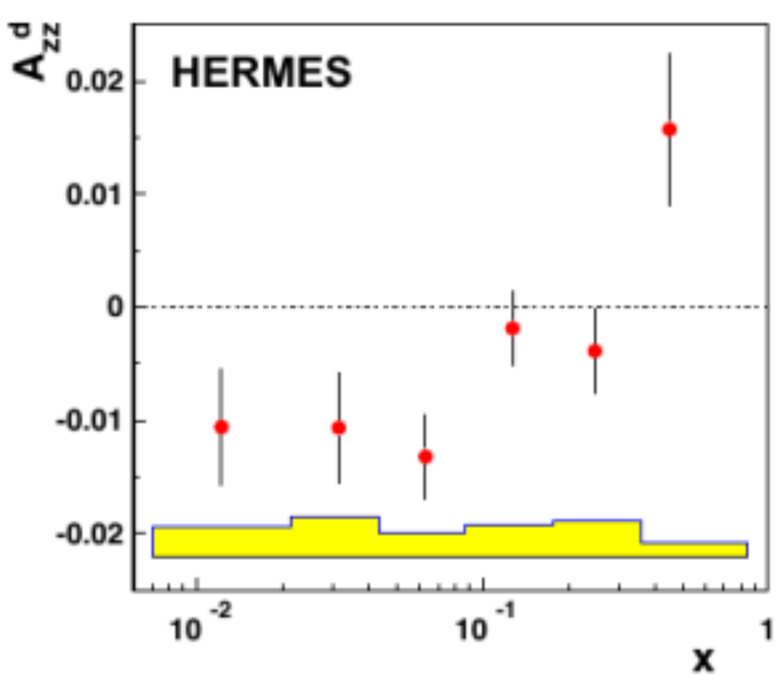
D. Keller

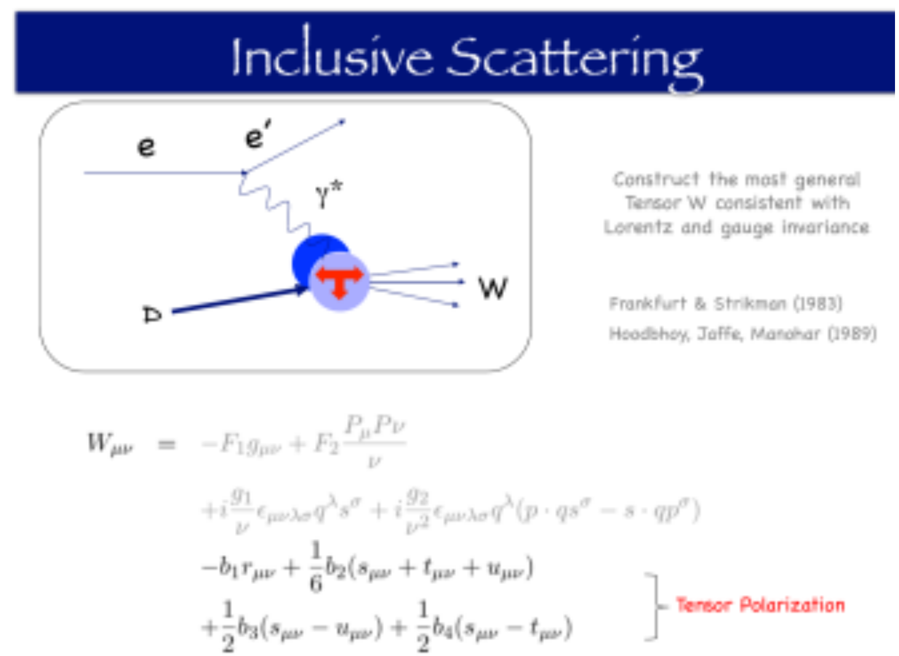
September, 2016

Contents

Solid Tensor Polarized Targets

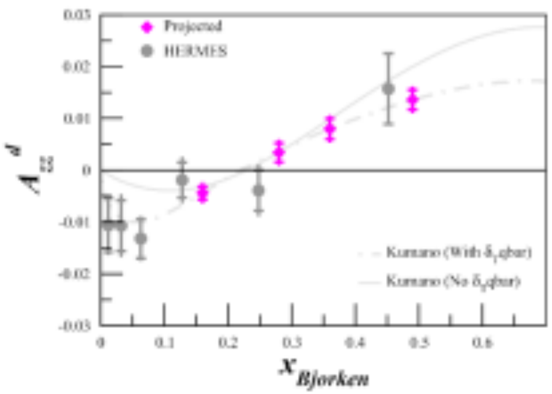
- Spin-1 structure functions (low for solid targets)
- Rather small asymmetries (10^{-3})
- False asymmetries ($\sim 2\delta\xi/fP_{zz}$)

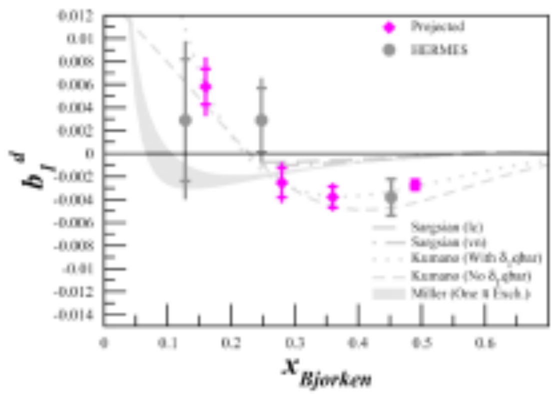




Some JLab C1 Approvals

E12-13-011: The Deuteron Tensor Structure Function b1 (Jlab Hall C)





$$b_1(x) = \frac{q^0(x) - q^1(x)}{2}$$

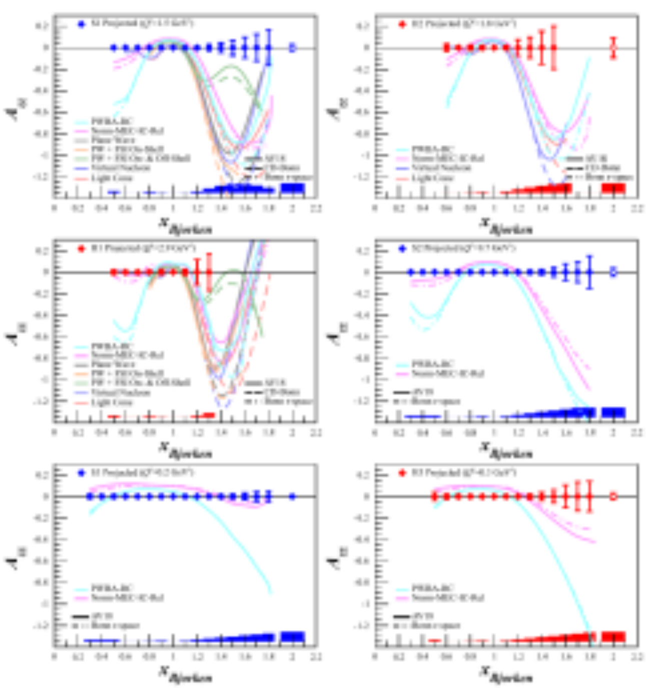
q^0 : Probability to scatter from a quark (any flavor) carrying momentum fraction x while the *Deuteron* is in state m=0

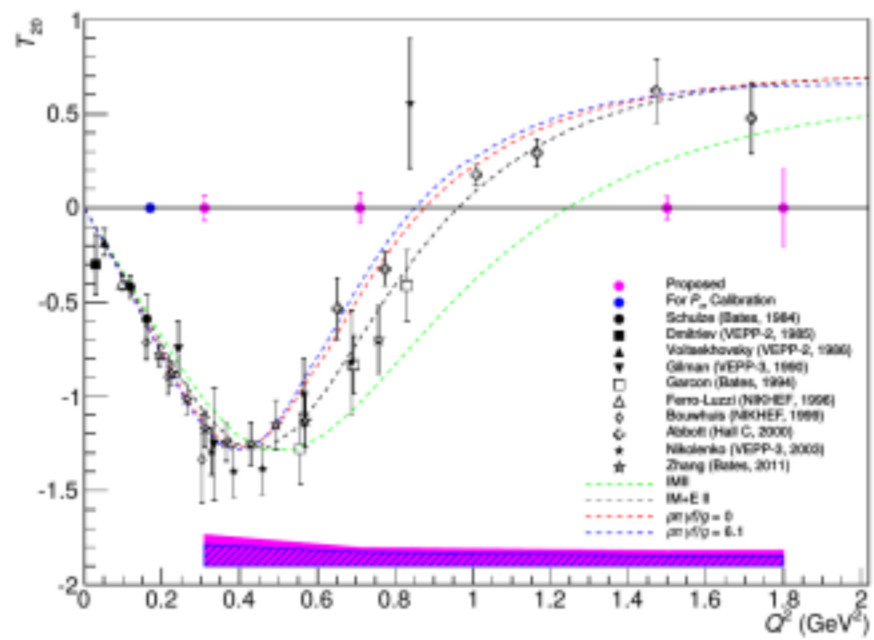
q^1 : Probability to scatter from a quark (any flavor) carrying momentum fraction x while the *Deuteron* is in state |m| = 1

$$A_{zz} = \frac{2}{fP_{zz}} \frac{\sigma_{\uparrow} - \sigma_0}{\sigma_0} = \frac{2}{fP_{zz}} \left(\frac{N_{\uparrow}}{N_0} - 1 \right)$$

$$b_1 = -\frac{3}{2} F_1^d A_{zz}$$

E12-15-005: Tensor Asymmetry in the Quasielastic Region (Jlab Hall C)



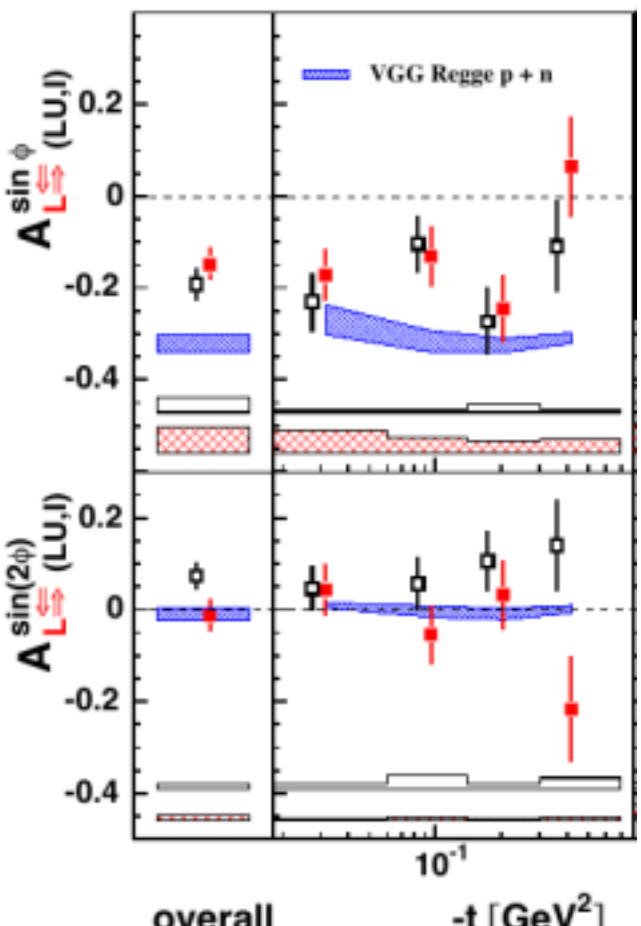


$$A_{zz} = \sqrt{2}\,[d_{20}T_{20} + d_{21}T_{21} + d_{22}T_{22}],$$

$$T_{20} = \frac{A_{zz}}{d_{20}\sqrt{2}} - \frac{d_{21}}{d_{20}}T_{21} - \frac{d_{22}}{d_{20}}T_{22}.$$

Also of Interest

- DVCS
- Drell-Yan



□ **unpolarized**

$\mathcal{R}e(\mathcal{H}_1)$

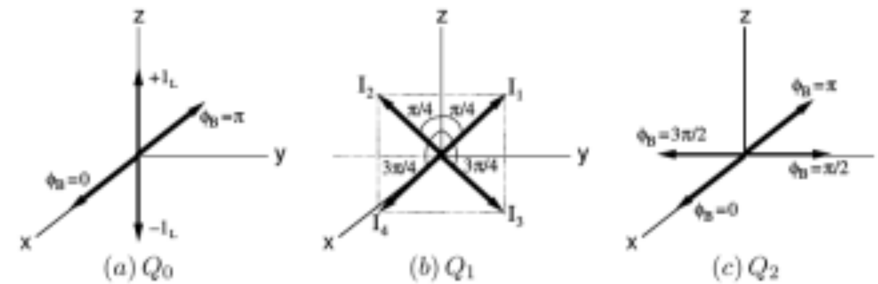
■ **tensor-polarized**

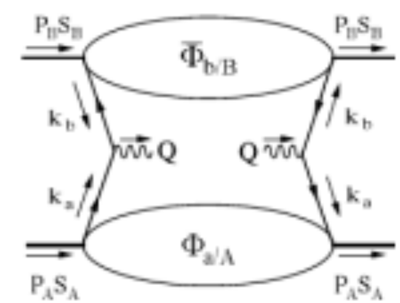
$\mathcal{R}e(\mathcal{H}_1 - \frac{1}{3}\mathcal{H}_5)$

Theoretical estimate on tensor-polarization asymmetry in proton-deuteron Drell-Yan process

S. Kumano[1,2,3] and Qin-Tao Song[1,3]

$W_{0,0}$, $V_{0,0}^{LL}$, $V_{0,0}^{TT}$, $V_{0,0}^{UQ_0}$, $V_{0,0}^{TQ_1}$, $W_{2,0}$, $V_{2,0}^{LL}$, $V_{2,0}^{TT}$, $V_{2,0}^{UQ_0}$, $V_{2,0}^{TQ_1}$, $U_{2,1}^{TU}$,
$U_{2,1}^{TQ_0}$, $U_{2,1}^{UT}$, $U_{2,1}^{LQ_1}$, $U_{2,1}^{TQ_2}$, $U_{2,1}^{TL}$, $U_{2,1}^{LT}$, $U_{2,1}^{UQ_1}$, $U_{2,2}^{UQ_2}$, $U_{2,2}^{TT}$, $U_{2,2}^{TQ_1}$, $U_{2,2}^{LQ_2}$,





Parton model for Drell-Yan
arXiv:1606.03149v2

DVCS A_{LZZ} (tensor asymmetry) sinϕ amplitude:

(no plot shown)

0.074 ± 0.196 ± 0.022

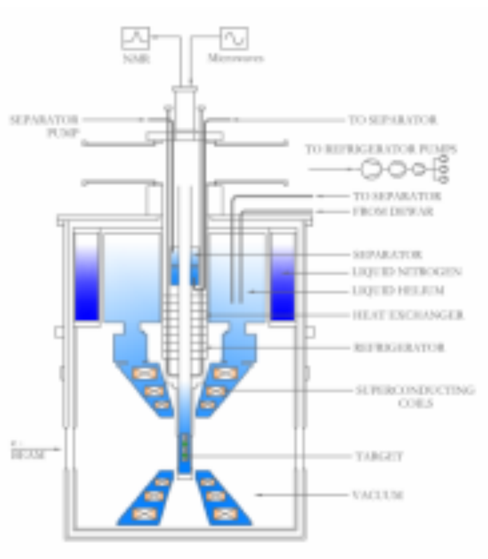
-t<0.06 GeV^2, 40% coherent,
dedicated data set with P_{zz}=-1.656 && P_z≈0

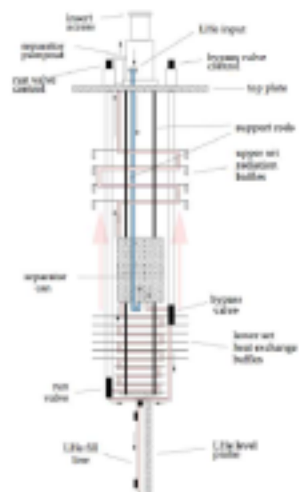
Challenges of a Solid Tensor Polarized Target

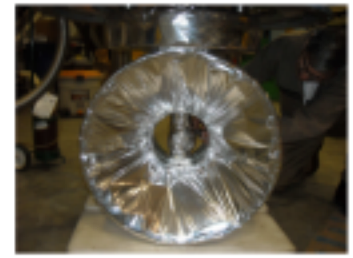
- High statistical precision requires high tensor polarization
- Time-dependent drifts are suppressed by the magnitude of polarization
- Tensor polarization of solid targets between 55-75% have been achieved below 300 mK (not for high intensity)
- Beam heating and radiation damage, limited to evaporation fridge with charged beam
- Maximize what can be achieved at 1K with Deuterated ammonia (need cold irradiation ~1K)
- Deuterated ammonia is complex with much about its DNP processes still to be learned

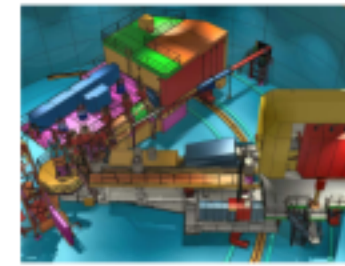
Experimental Environment

Solid Polarized Target Systems









- (A) ~100 nA
- (B) $10^{35} cm^{-2} s^{-1}$
- (C) Dilution factor f<50% (.3 for ND_3)
- (D) 5 T and 1 K

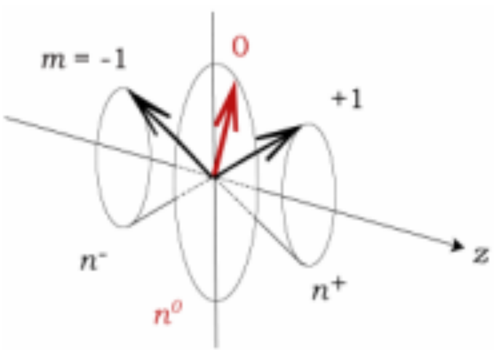
- Optimize Tensor Polarization for continuous charge beam experiments
- Do it in a way that the polarization can still be measured within reasonable error (<<10% relative)
- Test and check (room for corrections)

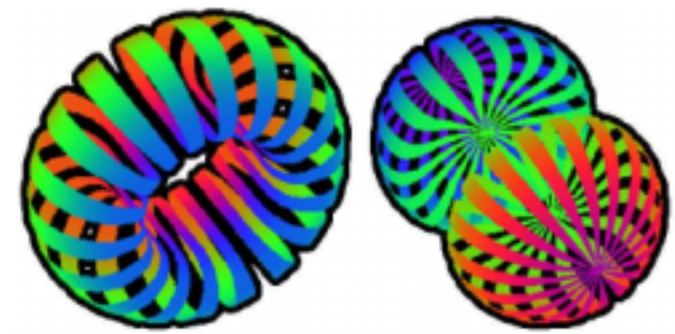
General Approach

- Start with a simplified Monte Carlo generated lineshape to study what the RF manipulated NMR should look like under tensor polarization optimization
- NMR phenomenology to mimic as much bulk behavior as possible
- Equations of motion under RF to fill in the blanks
- Model imposes constraints for NMR lineshape fitting for polarization measurements
- Improve model add in corrections as needed

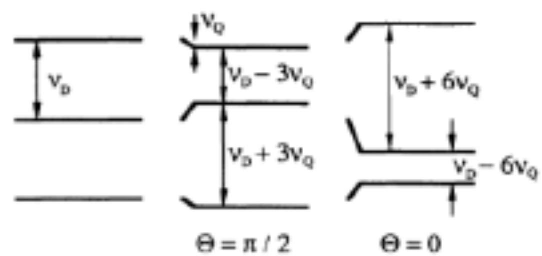
In the following examples the ND_3 was cold irradiated during at Jlab experiment, other examples are with d-but.

The Spin-1 Target

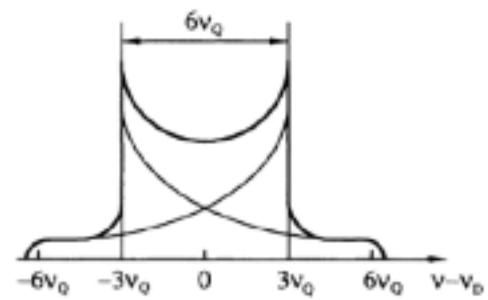


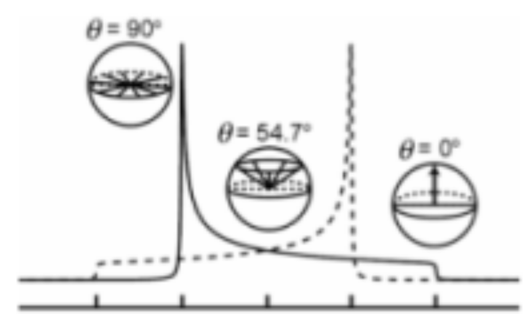


$$P = \frac{n_+ - n_-}{n_+ + n_- + n_0} \quad (-1 < P_z < 1)$$



$$P_{zz} = \frac{n_+ - 2n_0 + n_-}{n_+ + n_- + n_0} \quad (-2 < P_{zz} < 1)$$



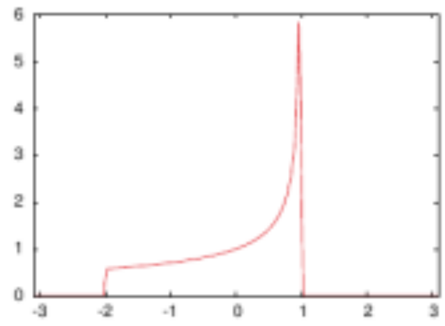


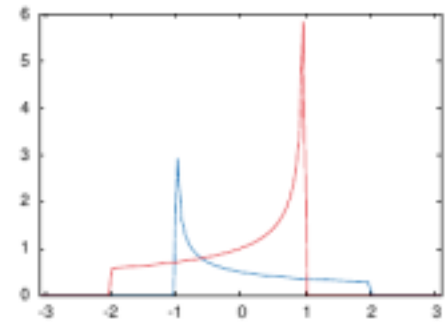
- Using Spin-1 (ND_3) Target
- Three Magnetic substates (+1,0,-1)
- Two Transitions ($+1 \rightarrow 0$) and ($0 \rightarrow -1$)
- Deuterons electric quadrupole moment eQ
- Interacts with electric field gradients within lattice

NRM Lineshape

$$P \propto \frac{1}{(1-R)^{1/2}}$$

$$-2 \leq R < 1$$





- $-2 \leq R \leq 2$
- $\Delta E_+ = E_0 - E_1$ with intensity I_+
- $\Delta E_- = E_1 - E_0$ with intensity I_-

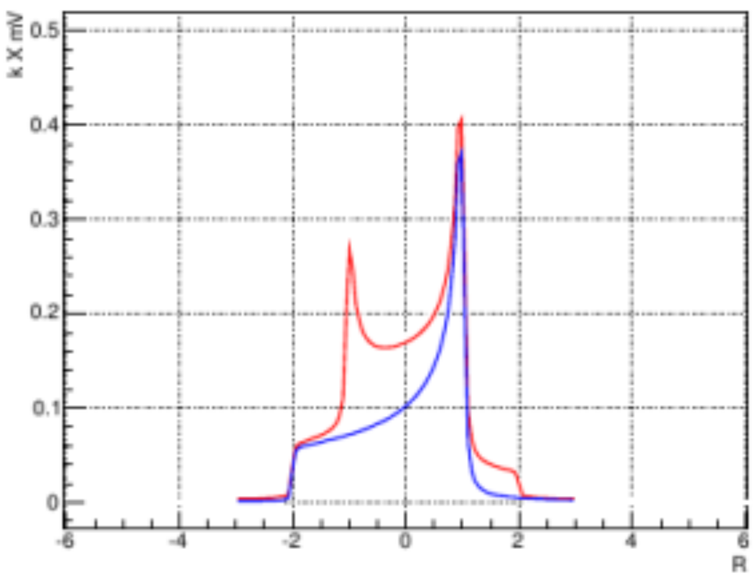
$$R = \frac{\omega - \omega_d}{3\omega_q}$$

- θ polar angle between the D bond and B_0
- ϕ azimuthal angle V_{ij} not symmetric
- η symmetry parameter (peak position)

$$\cos\theta = \sqrt{\frac{1 \pm R - \eta\cos 2\phi}{3 - \eta\cos 2\phi}}$$

$$\Delta E_\pm = \hbar\omega_d \mp 3\hbar\omega_q([3 - \eta\cos 2\phi]\cos^2\theta - [1 - \eta\cos 2\phi])$$

Homogeneous Broadening

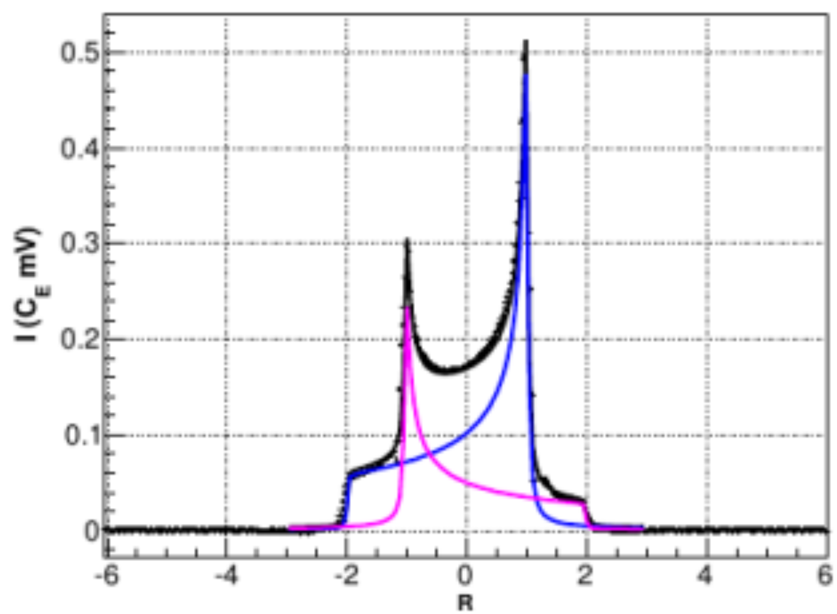


Distribution of $\omega_d \sim$ Lorentzian $\rightarrow$ intensity spectrum is a convolution of the density of states with a Lorentzian function

$$f(R) = G(R) \otimes \frac{\beta}{(1-R)^{1/2}}$$

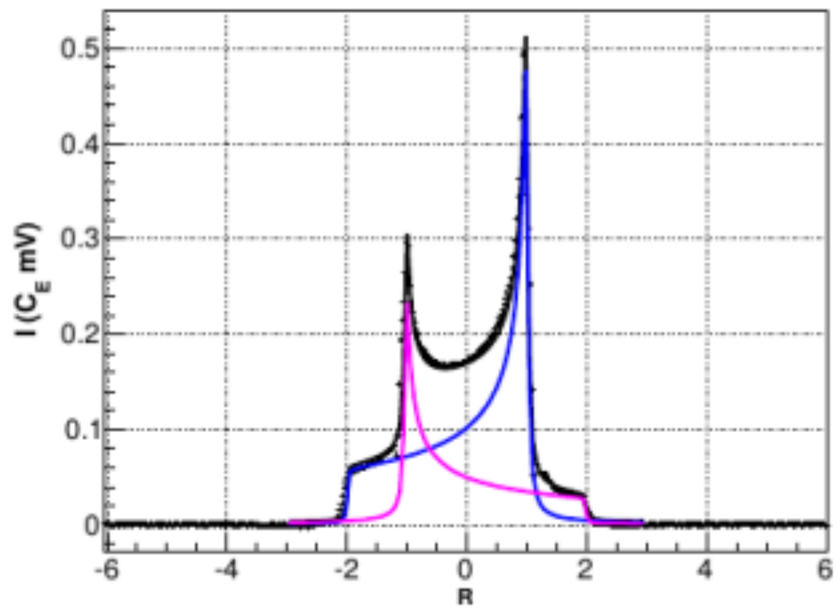
- Final lineshape is the sum of both absorption lines with effects from broadening
- Intensity of each transition is related to level population which is consistent and well known under Boltzmann equilibrium

Deuteron NMR Signal



- Vector and Tensor Polarization can be determined from the intensity of the individual absorption lines
- Fit and determine transition peak information

Measurement of DMR Signal



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

fit to ND_3

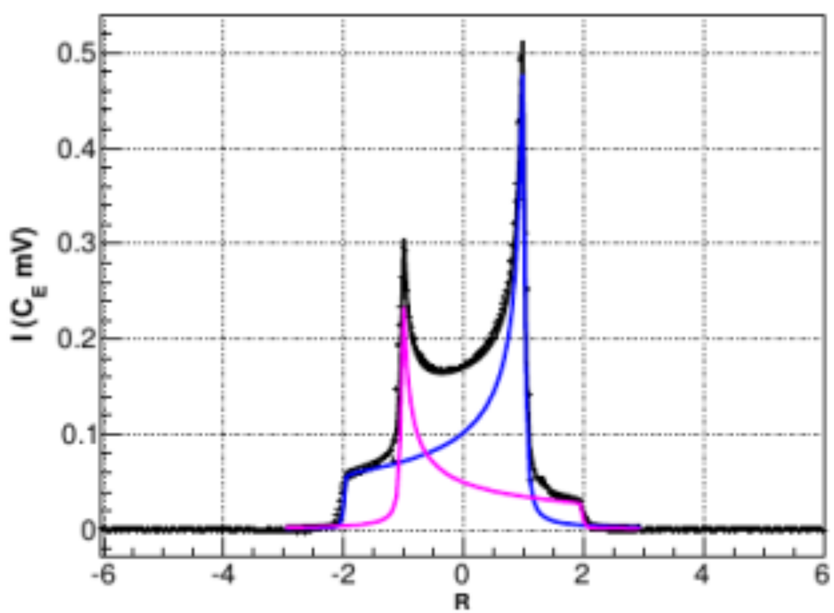
$\eta\cos 2\phi \sim 0.04$

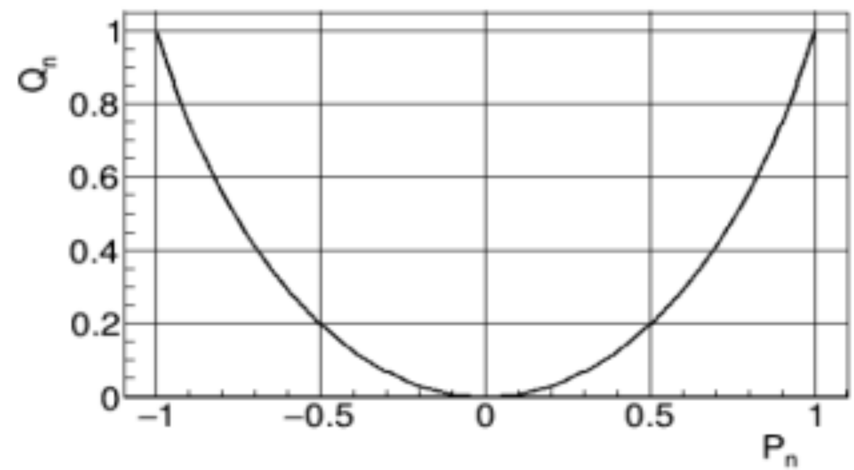
$$\mathcal{X}^2 = \sqrt{\Gamma^2 + (1-\epsilon R - \eta\cos 2\phi)^2} \qquad \mathcal{Y} = \sqrt{3-\eta\cos 2\phi}$$

$\Gamma \sim 0.05$

$$\cos\alpha = (1-\epsilon R - \eta\cos 2\phi)/\mathcal{X}^2 \qquad \epsilon = \pm 1$$

Measurement of DMR Signal





$$Q_n = 2 - \sqrt{4 - 3P_n^2}$$

- Under Boltzmann equilibrium a relationship between vector and tensor polarization always exists
- Under this same condition the Height of each peak maintains a relationship to each other that contains all polarization information
- The ratio of the peak intensities can be used to calculate relative population in each magnetic sub-level

$$P_n = \frac{2\hbar}{g^2\mu_N^2\pi N}\int_{-\infty}^{\infty}\frac{3\omega_Q\omega_D}{3R\omega_Q+\omega_D}\chi''(R)dR$$
$$= \frac{1}{C_E}\int_{-\infty}^{\infty} I_+(R) + I_-(R)dR,$$

$$Q_n = (I_+ - I_-)/C_E$$

Measurement of DMR Signal

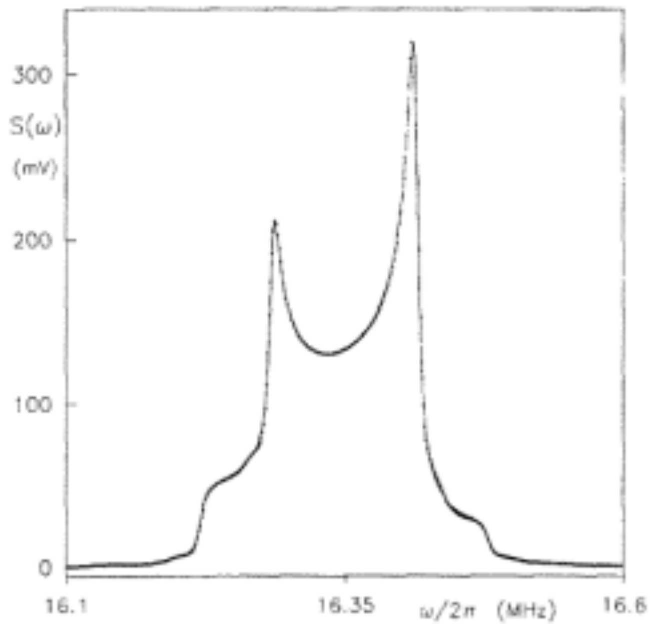


Fig. 7. An enhanced signal of 44% polarization (circles) with the fitted curve superimposed (line).

$$n_+ \approx \mathcal{N} e^{\beta\hbar\omega_d}\{1 + \tfrac{2}{5}(\beta\hbar\omega_q)^2\},$$
$$n_- \approx \mathcal{N} e^{-\beta\hbar\omega_d}\{1 + \tfrac{2}{5}(\beta\hbar\omega_q)^2\},$$
$$n_0 \approx \mathcal{N}\{1 + \tfrac{8}{5}(\beta\hbar\omega_q)^2\},$$

$$P_n = \frac{n_+ - n_-}{n_+ + n_- + n_0} = \frac{r^2 - 1}{r^2 + r + 1} + \mathcal{O}((\beta\hbar\omega_q)^2)$$

$$Q_n = \frac{n_+ - 2n_0 + n_-}{n_+ + n_- + n_0} = \frac{r^2 - 2r + 1}{r^2 + r + 1} + \mathcal{O}((\beta\hbar\omega_q)^2)$$

C. Dulya, et al., NIM A 398 109-125 (1997)

A line-shape analysis for spin-1 NMR signals

The Spin Muon Collaboration (SMC)

- The asymmetry 'r' is a good parameter to use for determining the polarization when related to the lineshape
- This relationship is established through intensity factors
- This factor can be established by fitting the absorption function to establish the asymmetry under Boltzmann equilibrium

Establish Calibration

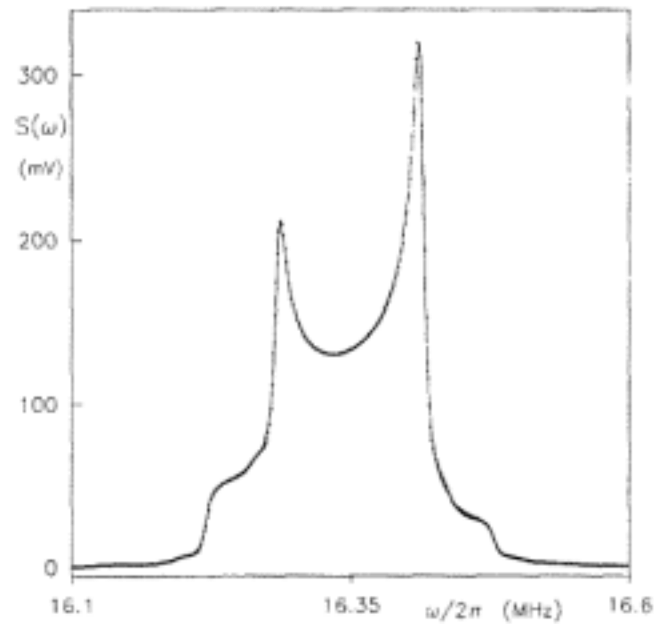
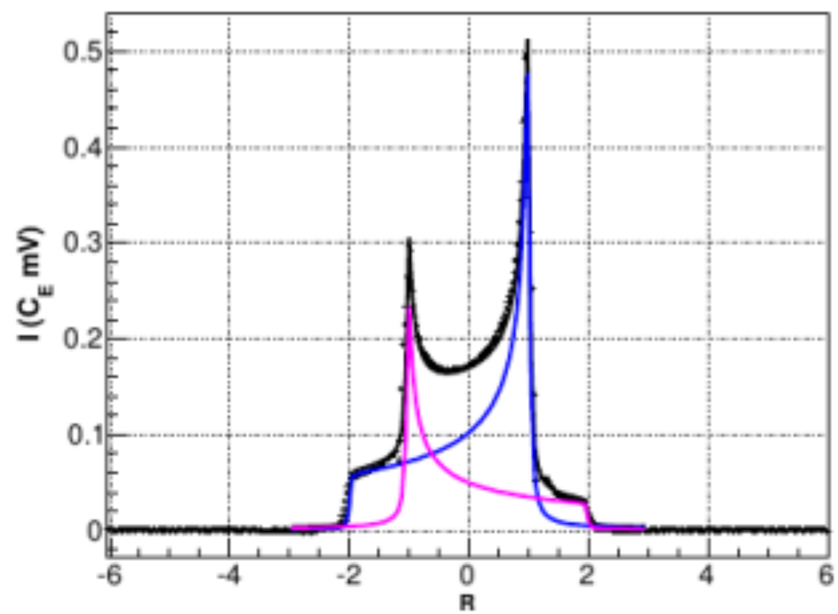
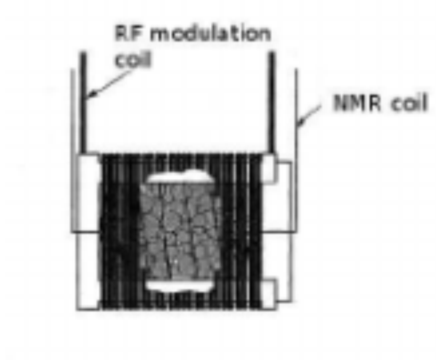


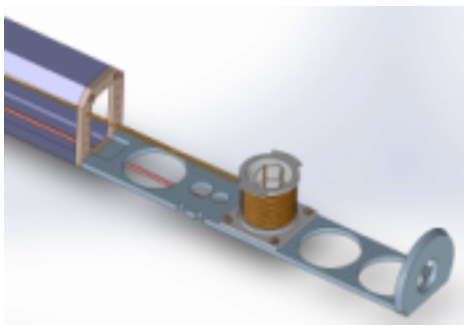
Fig. 7. An enhanced signal of 44% polarization (circles) with the fitted curve superimposed (line).

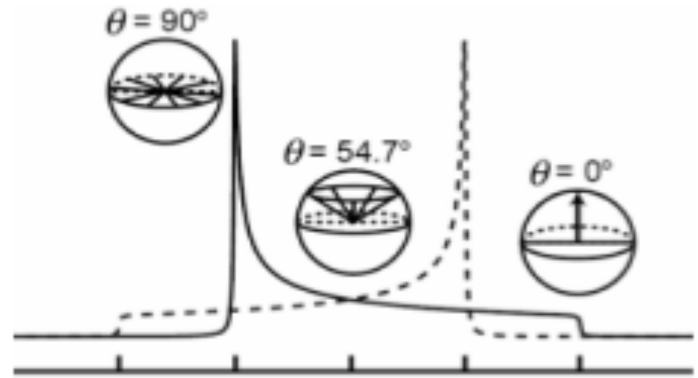


- For cleanest measurement use multiple TE
- With multiple peak height fits under Boltzmann equilibrium
- Support Vector Machine background suppression with single\baselines training

RF Manipulation

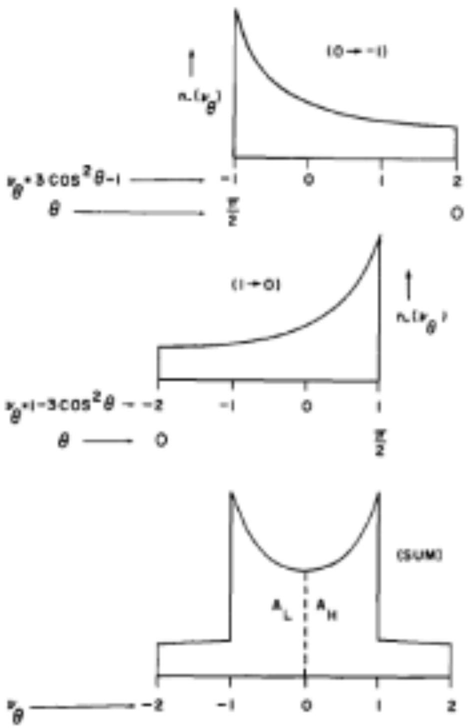






- RF irradiation at the Larmor frequency induces transitions between m=0 and other energy levels
- RF induced transitions at a single θ has a resulting effect on two positions in the line R and $-R$ through conservation of energy
- This can be implemented to shrink one transition lines area and enhancing the other resulting in tensor polarization manipulation

Previous Work



THE FROZEN SPIN ORIENTATION OF DEUTERIUM NUCLEI IRRADIATED AT RADIO-FREQUENCIES

P.P.J. DELHEIJ, D.C. HEALEY and G.D. WAIT

TRIUMF, 4004 Wesbrook Mall, Vancouver, BC, Canada V6T 2A3

With eqs. (11) and (13) the changes in polarization and alignment respectively become:

$$\Delta P = P - P^0 = \Delta I / C_{cal}, \quad (20)$$

$$\Delta A = A - A^0 = 3\Delta I / C_{cal}, \quad (21)$$

which leads to:

$$\Delta A = 3\Delta P. \quad (22a)$$

- de Boer W. et al. Phys. Lett. B 46, 143 (1975)
- W. Meyer and E. Schilling Bonn-he-85-06
- W. Meyer et al. 4th PSTP B Honnef 165 (1984)
- P. Delheij et al. NIM A 251 498 (1986)
- G. R. Smith NIM A 254 263 (1987)

Previous Work

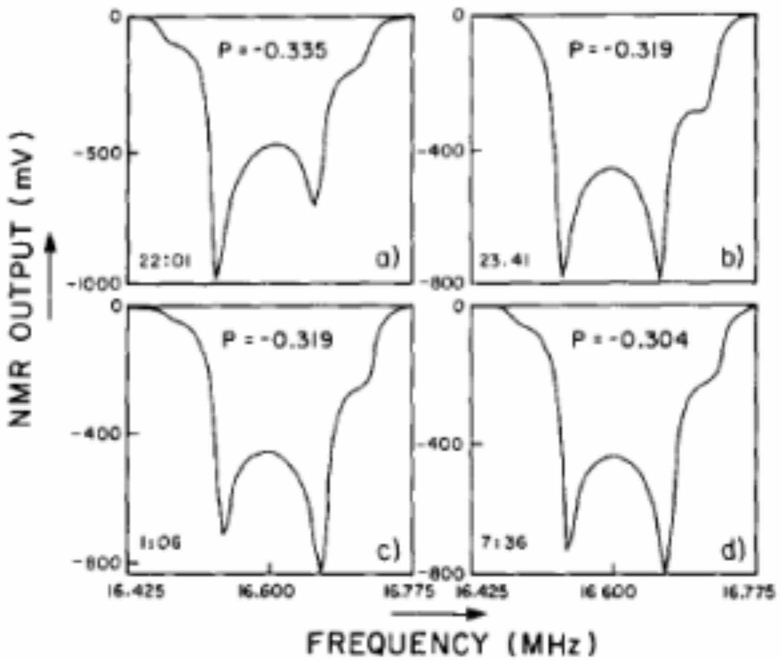
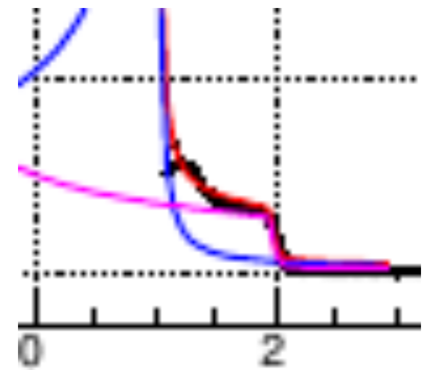


Fig. 5. Some NMR spectra are shown for the procedure in which the pedestal of the (1 → 0) transition was burnt (b) for 100 min. Parts (c) and (d) result from decay in a magnetic field of 1.25 T between the measurements. For each part the polarization *P* and the time of day is indicated.



$\Delta P_{zz} = -3\Delta P_z$

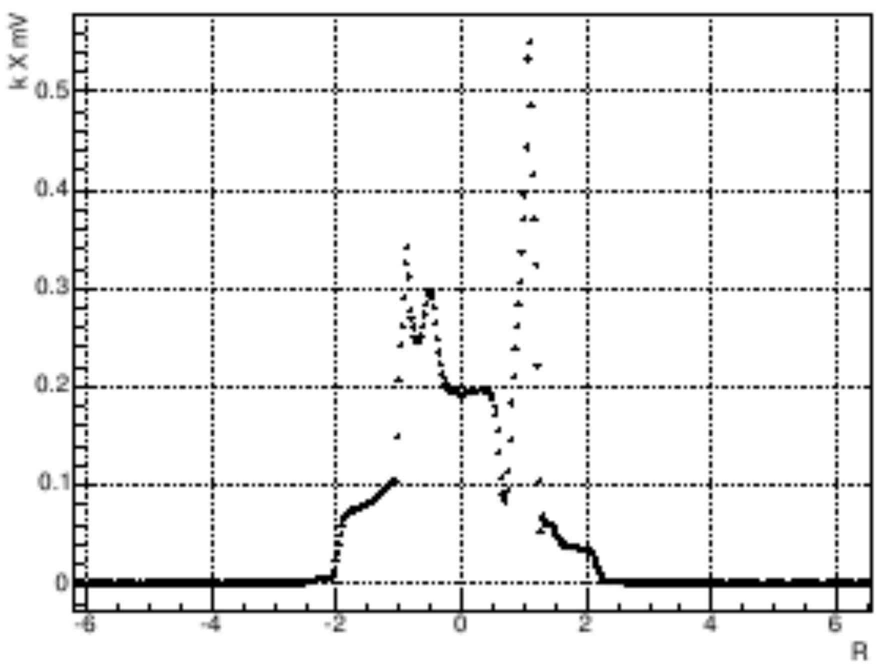
- $\delta\Delta P_{zz} = 3\delta(P_z - P'_z) \sim 20\%+$
- No-broadening
- Losses from excess RF

- Traditionally measurements and methods never worked good enough to use in an scattering experiment
- Spectral diffusion, error in formula, error in approximation

Modern Effort

- Study Optimization Analytically
- Develop Simulated Lineshape under RF
  - Empirical info from RF-power profile and Spectral diffusion
  - Rate Eq for overlap ratio
  - Generate theoretical lineshape manipulated by RF
- Develop fitting procedure for measurement
  - Unique constraints for overlapping regions are provided by MC
  - Fit semi-saturated (optimized d-Ammonia)
  - Test measurements with specialized NMR and scattering experiments
- Further Optimized Enhancement
  - Slow Perpendicular Rotation with semi-saturating RF
  - Heavily Reliant on MC for measurements
  - Tested with d-but. but not yet for ammonia

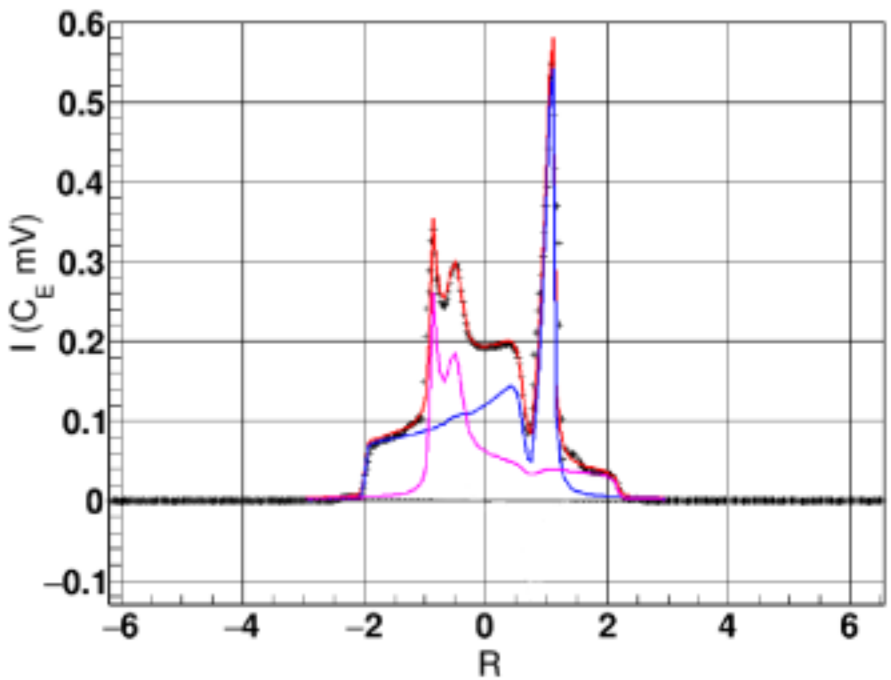
Bulk Behavior from Data into MC



- Distortions to the lineshape in the from of a Voigt
- Changes clearly at *R* and -*R* and thats it
- Spectral diffusion seen but only at RF location during recovery

- Extract parameters directly from data
- RF manipulation specific to coil and power
- Modulation still used Voigt over region
- Saturation simplifies
- Semi-saturation requires rate equations at *R*

Bulk Behavior from Data into MC



- Distortions to the lineshape in the from of Voigt
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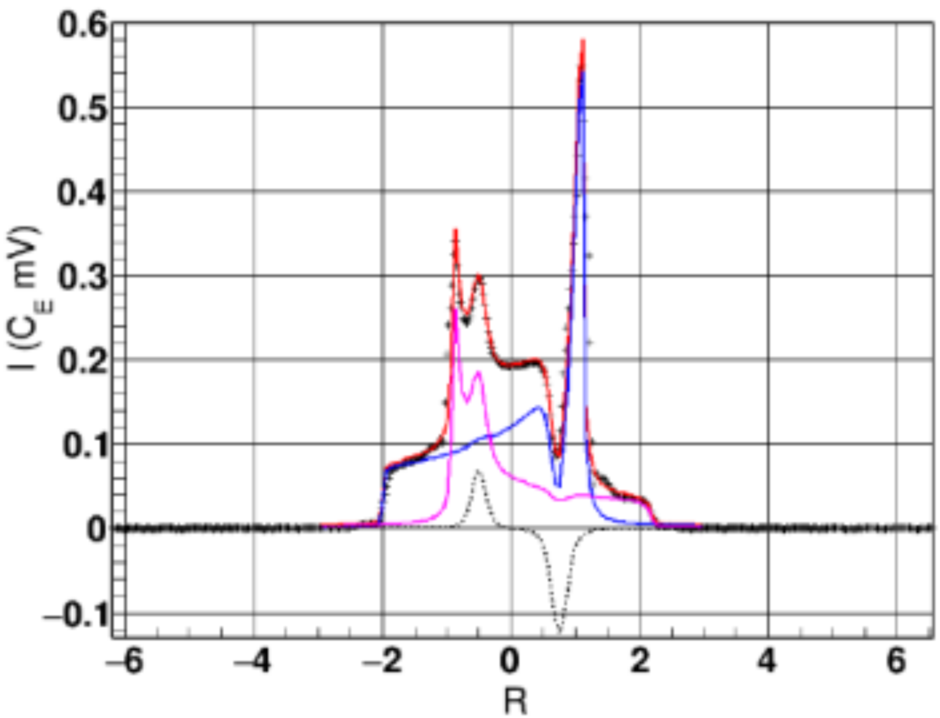
- RF manipulation specific to coil and power
- Modulation still used Voigt over region
- Saturation simplifies
- Semi-saturation requires rate equations at *R*
- Results for bulk data and MC must be near identical

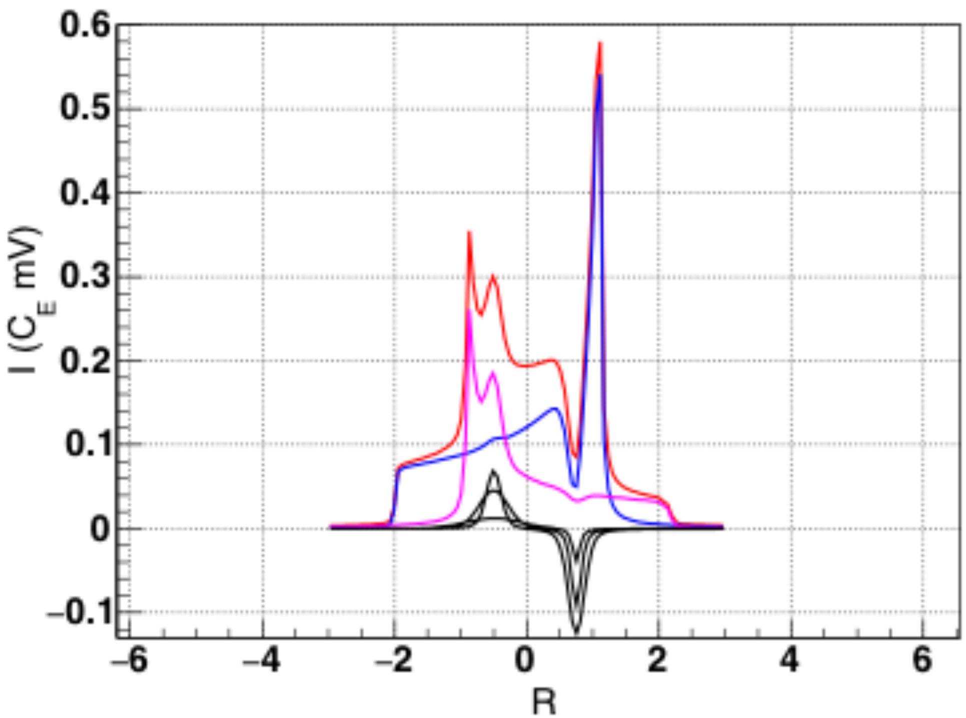
Bulk Behavior from Data into MC



- Distortions to the lineshape in the from of Voigt
- Changes clearly at *R* and -*R* and thats it
- Spectral diffusion seen but only at RF location during recovery

- Extract parameters directly from data to mimic in MC
- Two Voigts at *R*
- Two Voigts at -*R*
- Approximate Equal widths
- Add in recovery behavior spectral diffusion around *R*

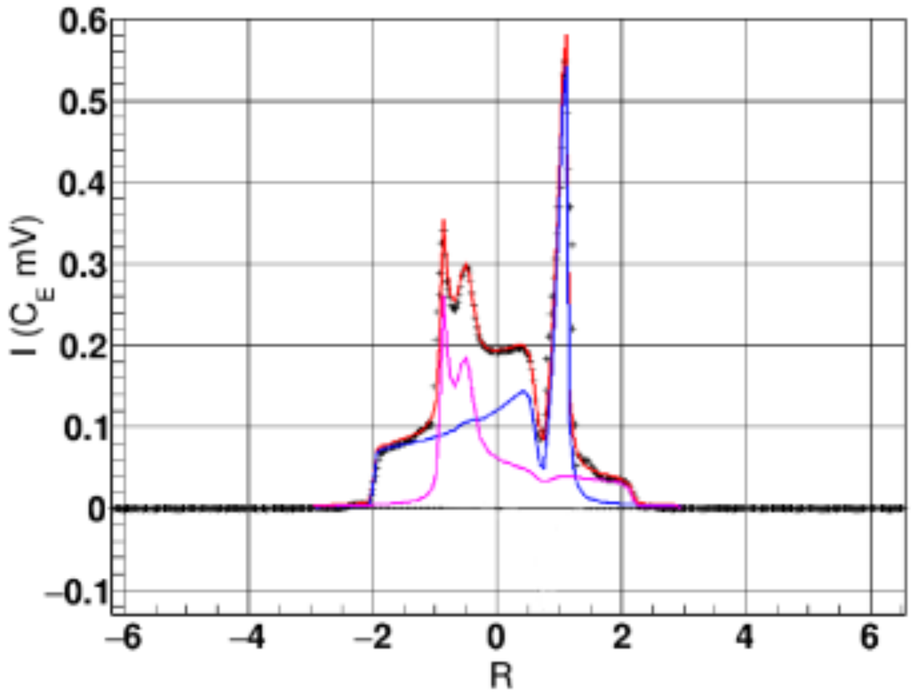
Bulk Behavior from Data into MC



- Distortions to the lineshape in the from of Voigt
- Changes clearly at *R* and -*R* and thats it
- Spectral diffusion seen but only at RF location during recovery

- *R* from the RF hole fills in
- And -*R* broadens from diffusion and spreads within the line
- Add in diffusion constant for completeness
- Bulk behavior simulated very well
- But what about intensities?

Need to Model Overlap Behavior



- Use Model based on simplified solid effect
- Simplest most sensible place to start
- This style of model is only weakly relying on the rate equations
- W. Meyer et al., NIM 526 12-21 (2004) possible Differential Solid Effect for warm irradiated d-ammonia

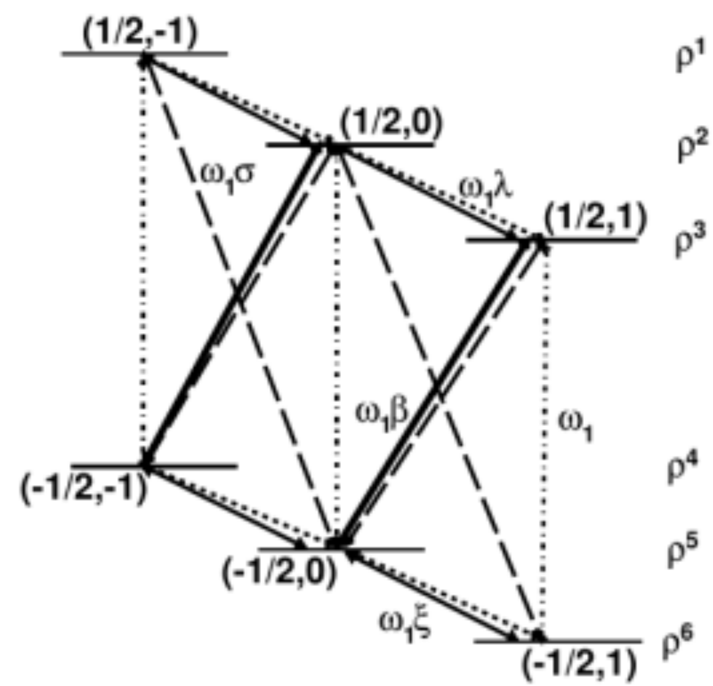
- Find $r(R)=I_+(R)/I_-(R)$ for all possible intensities
- Generate a lineshape and model from results
- Improve as needed

Find Overlapping Ratio at *R*

L. JiZhi, Commun. Theor. Phys. 31 619 (1999)

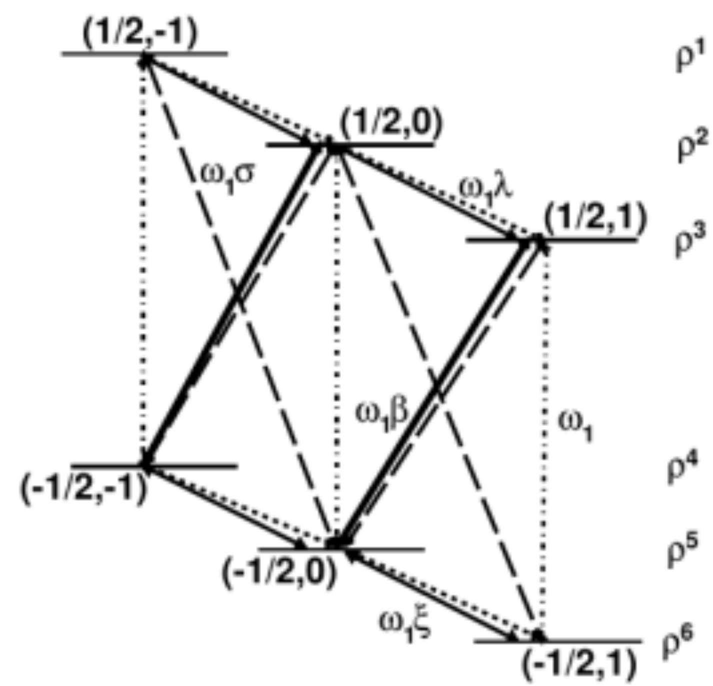
$$2T_{1e}\frac{d\rho^i}{dt} = \sum_{j\neq i}(\rho_j\omega_{ji} - \rho_i\omega_{ij})$$

$$\begin{aligned}
\dot{\rho}^1(\mathbf{B}_\mu,\mathbf{B}_\nu) &= \xi\omega_1(\rho^2-\rho^1)\\
\dot{\rho}^2(\mathbf{B}_\mu,\mathbf{B}_\nu) &= \beta\omega_1(\rho^4-\rho^2)+\xi\omega_1(\rho^3-2\rho^2+\rho^1)\\
\dot{\rho}^3(\mathbf{B}_\mu,\mathbf{B}_\nu) &= \beta\omega_1(\rho^5-\rho^3)+\xi\omega_1(\rho^2-\rho^3)\\
\dot{\rho}^4(\mathbf{B}_\mu,\mathbf{B}_\nu) &= \beta\omega_1(\rho^2-\rho^4)+\xi\omega_1(\rho^5-\rho^4)\\
\dot{\rho}^5(\mathbf{B}_\mu,\mathbf{B}_\nu) &= \beta\omega_1(\rho^3-\rho^5)+\xi\omega_1(\rho^4-2\rho^5+\rho^6)\\
\dot{\rho}^6(\mathbf{B}_\mu,\mathbf{B}_\nu) &= \xi\omega_1(\rho^5-\rho^6).
\end{aligned}$$



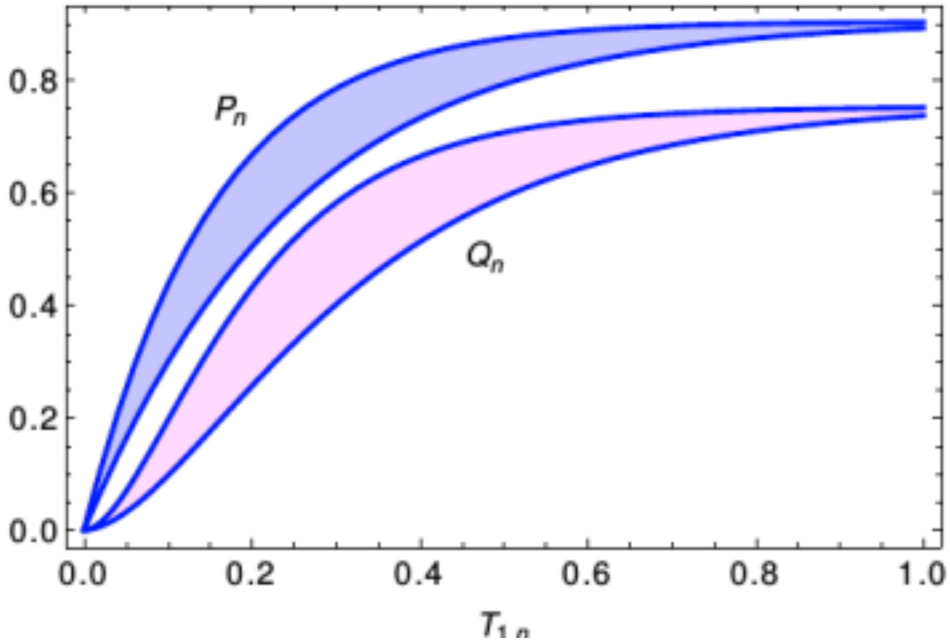
Find Overlapping Ratio at *R*

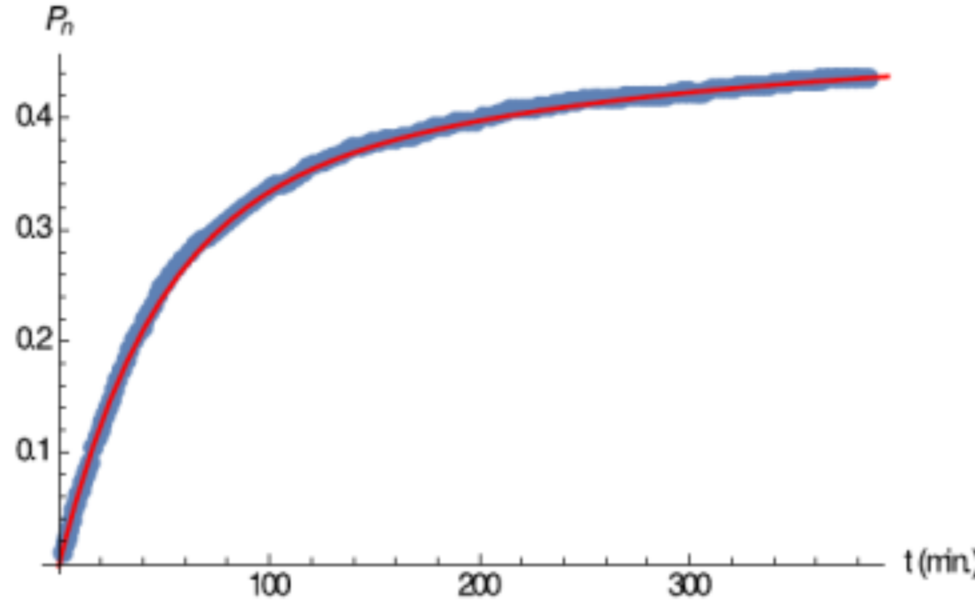
- Re-derive set of differential equation at RF position
- Workout equations in terms of polarizations and decay times
- Solve Numerically
- Find ratio of intensities at *R*



$$\dot{\rho}^1(\mathbf{B}_\nu,\mathscr{R}) = \xi\omega_1(\rho^2(\mathscr{R})-\rho^1(\mathscr{R}))$$
$$\dot{\rho}^2(\mathbf{B}_\nu,\mathscr{R}) = \xi\omega_1(\rho^1(\mathscr{R})-\rho^2(\mathscr{R}))$$
$$\dot{\rho}^3(\mathbf{B}_\nu,\mathscr{R}) = 0$$
$$\dot{\rho}^4(\mathbf{B}_\nu,\mathscr{R}) = \xi\omega_1(\rho^5(\mathscr{R})-\rho^4(\mathscr{R}))$$
$$\dot{\rho}^5(\mathbf{B}_\nu,\mathscr{R}) = \xi\omega_1(\rho^4(\mathscr{R})-\rho^5(\mathscr{R}))$$
$$\dot{\rho}^6(\mathbf{B}_\nu,\mathscr{R}) = 0.$$

Numerical Solutions



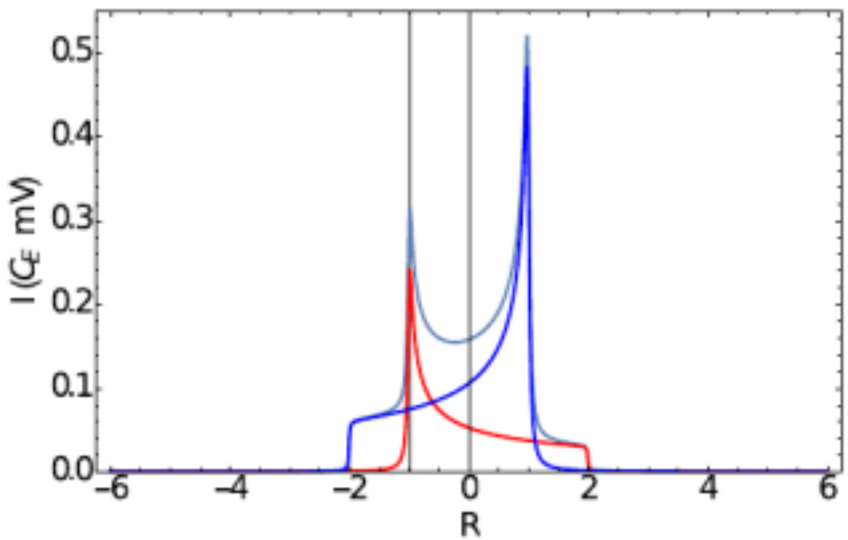


- Check solutions give similar results to previous publications without the coil RF
- Make sure things make sense in the relationship between *Q* and *P*
- Setup ramp-up and decay timing for material of interest

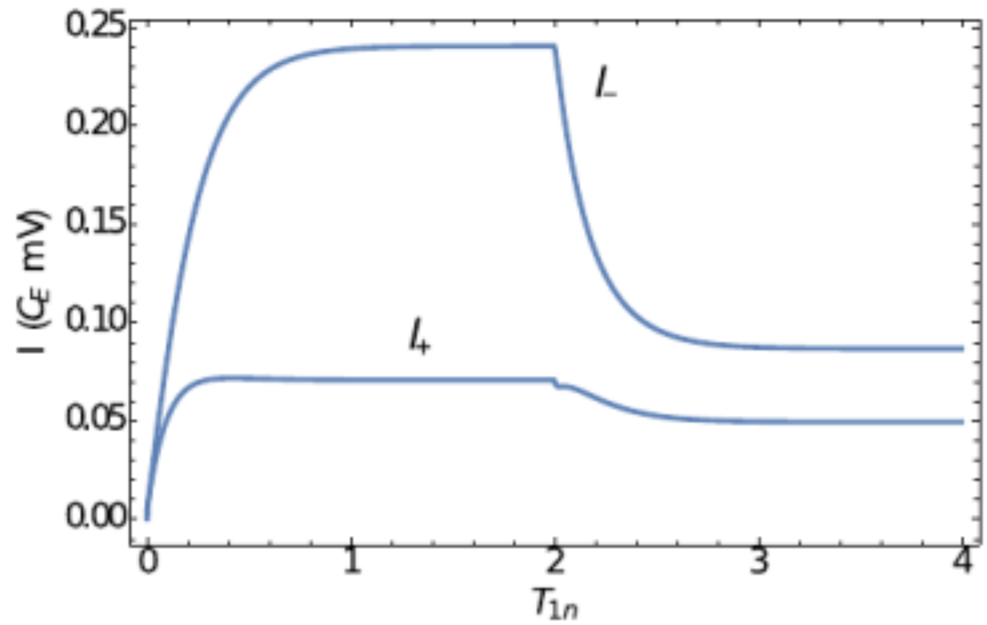
- Parameterization from build-up data using NDE fit or tune by qualitative overlap
- Extract T_{1e}, P_0, and *C* from ND_3 NMR data
- Make time scale correspond to relaxation rate T_{1n}

Tensor Enhancement Mechanism

Tensor Enhancement Mechanism for single position



Selective Semi-saturation : Use power appropriate for position optimizing tensor polarization for all *R*

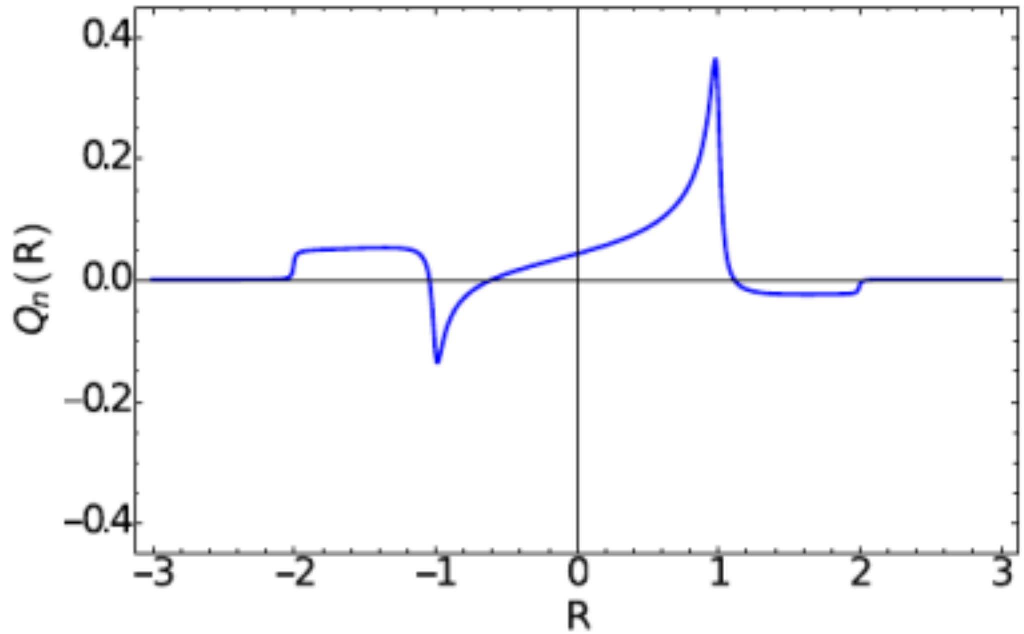


For peak Semi-saturation significant enhancement occurs by reduction of negative tensor polarization at *R* as well as adding to positive tensor polarization at -*R*

- Total target tensor polarization enhancement occurs when negative tensor polarization is minimized and positive tensor polarization is maximized
- Greater initial polarization provides greater initial tensor but semi-saturation adds more enhancement for lower polarized samples
- Ultimately just need to RF two places in one transition for best enhancement

Tensor polarization in the line

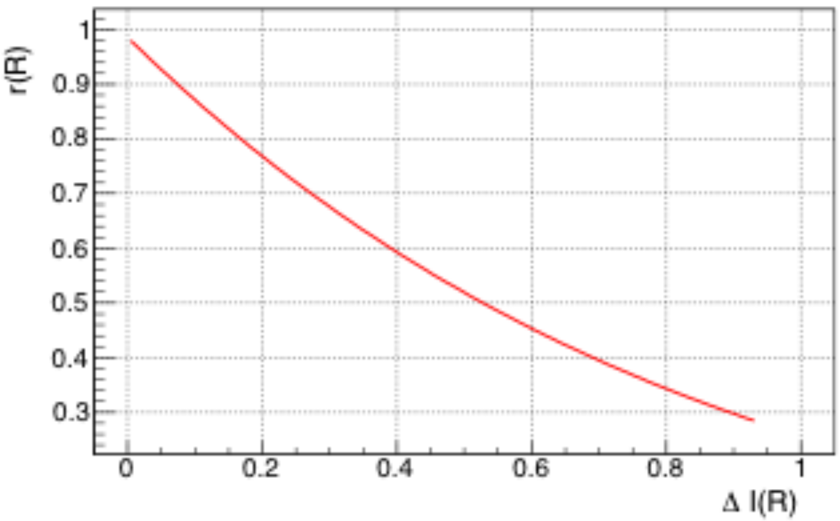
Full target vector polarization of ~40%



Tensor polarization $Q_n(R)$ within the NMR line

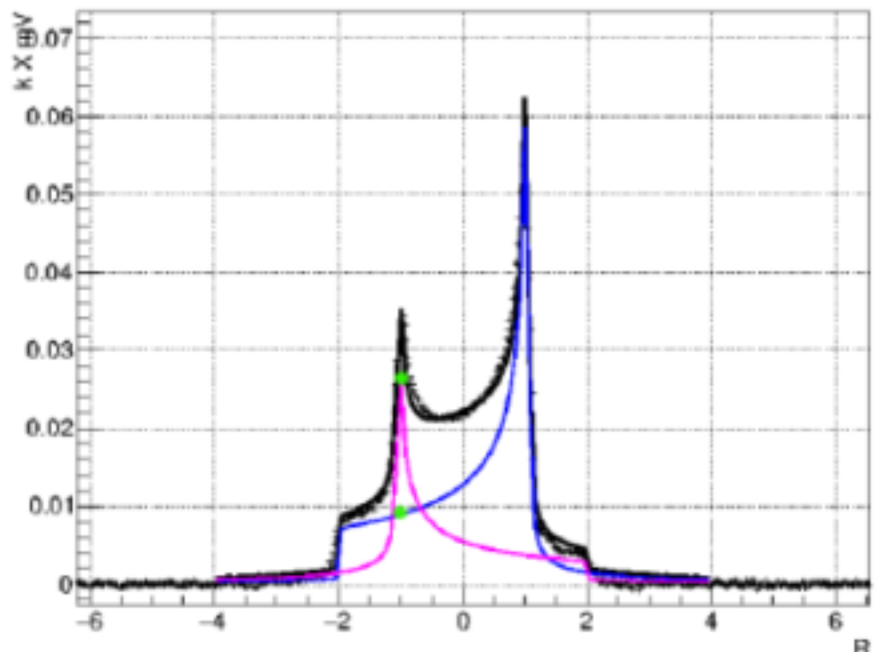
- Enhancement occurs when negative $Q_n(R)$ is minimized and positive $Q_n(R)$ is maximized
- Optimize in Monte Carlo by moving Voigt around and modulating RF
- In reality just single position at small peak with nearly full saturation at small pedestal is best

Resulting Model Predictions for *r(R)*



$$r = \frac{I_+}{I_-} \rightarrow r(R) = \frac{I_+(R)}{I_-(R)}$$

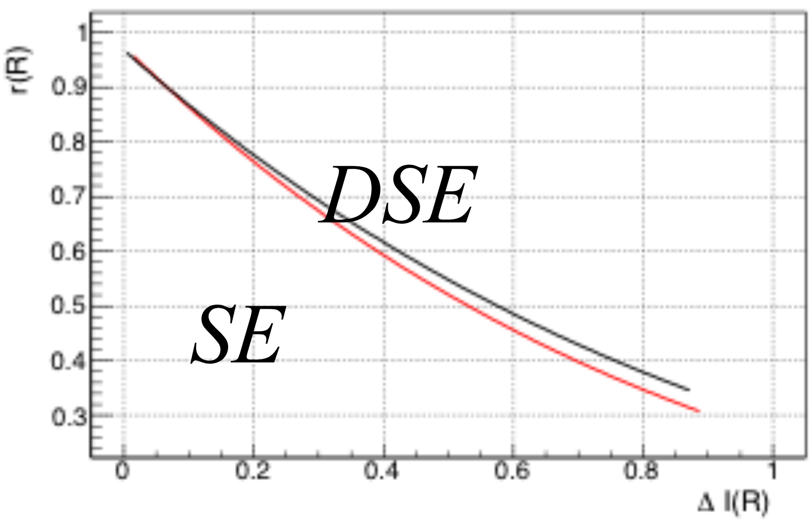
ΔI=I(R)-I′(R)

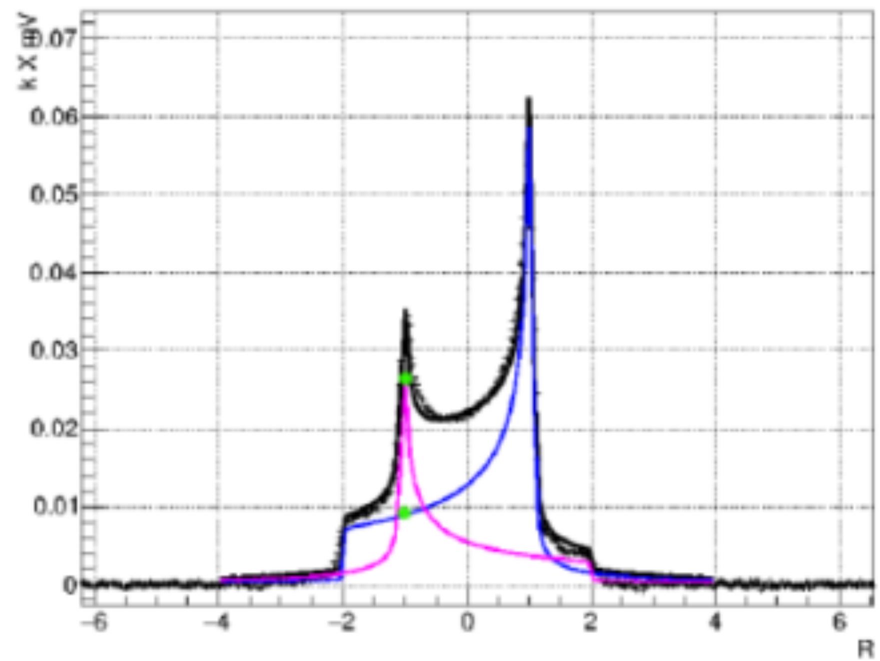


Examples for initial vector polarization 42%

- Find resulting family of function relating *r(R)* to *ΔI* for all polarizations
- Can calculate intensity for overlapping absorption lines for any polarization and any RF strength
- Results lead to an optimized *ΔI* easily determined by NMR measurements
- Final family of functions are used in Monte Carlo and fitting constraint

Polarization Mechanism Sensitivity



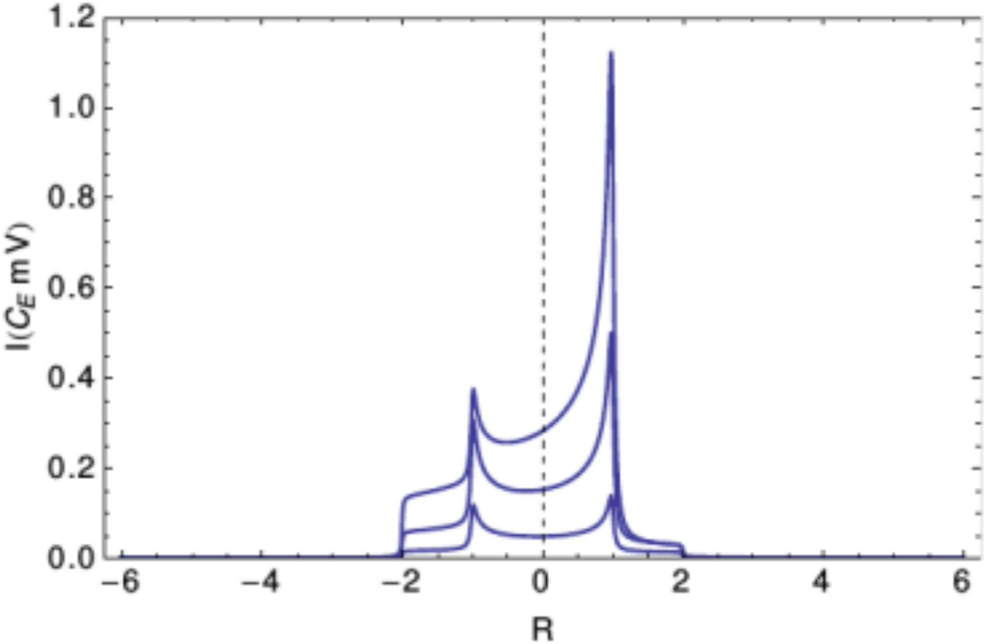


$$r = \frac{I_+}{I_-} \to r(R) = \frac{I_+(R)}{I_-(R)}$$

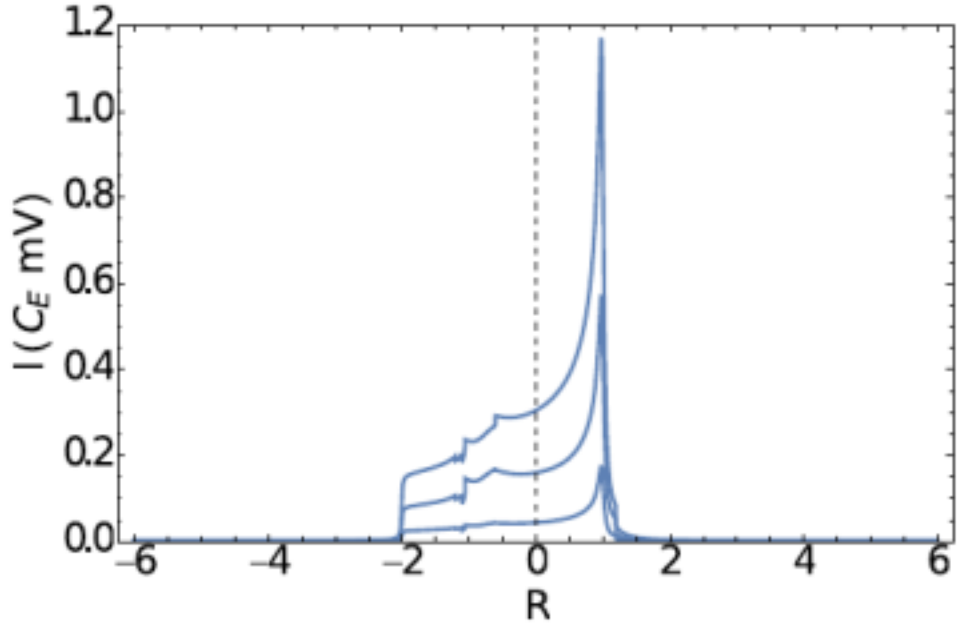
$$\Delta I = I(R) - I'(R)$$

- Preliminary look at Solid Effect and Differential Solid Effect
- Only slight variation in ratio leading to <0.4% variation total area of at Optimized *ΔI*
- Can be used in Monte Carlo and fitting constraint

MC Optimal Lineshape



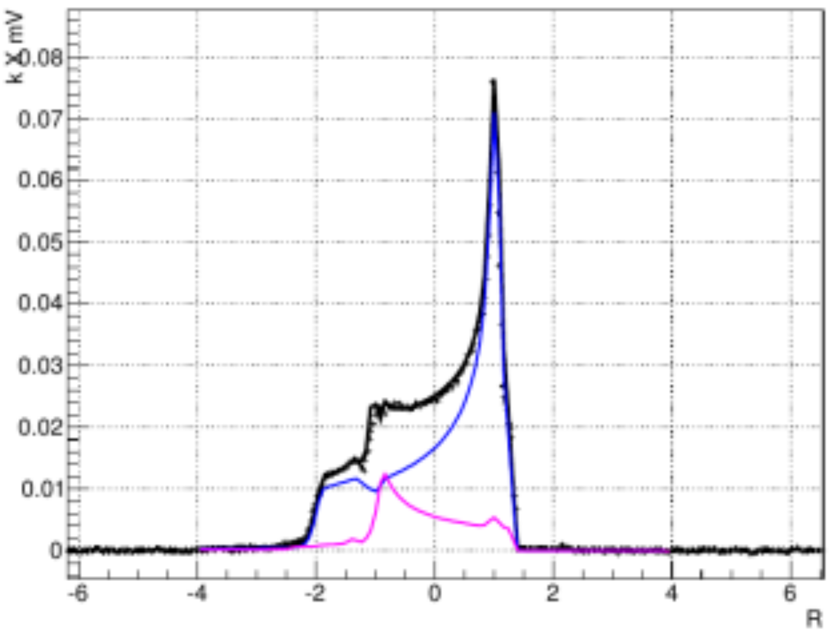
Simulated Examples of regular lineshape
(13,42,78%)



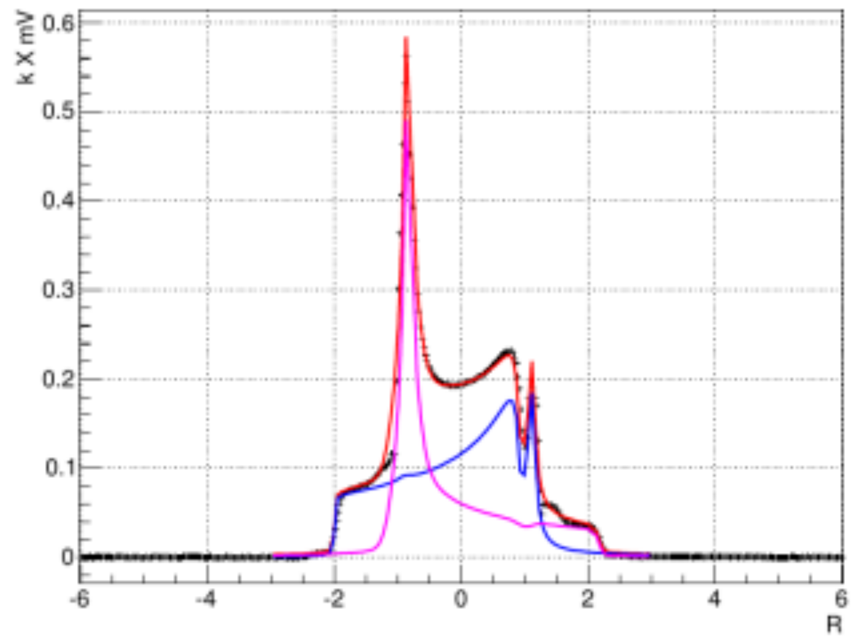
Examples Optimized Tensor Polarization
Examples (1.3→5.4,13.6→23.8,52→58%)

- Theoretical lineshape for enhancement
- Ideal line generated using modulated Voigt
- Relative RF power varied for each frequency

Some Preliminary Comparison to Real NMR Data



MC overlap with d-but. NMR experimental points (Pn=51→45,Qn:20→31%)



MC with fit and d-but. NMR experimental points (Pn=48→46,Qn:18→6%)

- MC and fitting contains same information
- These are very clean examples, encouraging, inconclusive
- Still need much confirmation on the overlap portion

Tests and Checks

- Specialized NMR studies to come (S-MAS) (hole-splitting)
- Lineshape vs Scattering polarization extraction T_{20} measurements (Jlab E12-15-005, HIGS P-12-16)
- Add in additional polarization mechanisms
- Small corrections to r(R) maybe all that is needed here

Conclusion

- Developed a simulation and fitting method
  - Incorporates bulk information (diffusion, recovery,..)
  - Only lightly depends on a SE-model (single point)
  - Further expansion of modeling are interesting (necessary?)
  - Polarization mechanisms, molecular dynamics, simulation in full signal, frequency dependence

- Lots more work to come
  - Need experimental verification
  - Cold(~1K) irradiated ND3
  - Experimental and theoretical development for warm and cold irradiated ND3
  - All the same stuff for rotation