Polarization Optimization and Measurement for Solid Spin-1 Targets
for the 22nd International Spin Symposium

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- What Types of Experiments
- Spin-1 Nuclear Magnetic Resonance
- RF Manipulated Lineshape
- Optimization of Tensor Polarization
- Where we are and where we are going
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

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

\[ A_{zz} = \frac{1}{f_{Pzz}} \frac{\sigma_1 - \sigma_0}{\sigma_0} = \frac{3}{2} \frac{N_1 - N_0}{N_0} \]

\[ b_1 = -\frac{3}{2} F_1^t A_{zz} \]
Also of Interest

- DVCS
- Drell-Yan

Parton model for Drell-Yan
arXiv:1606.03149v2
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

- 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)

- (A) $\sim 100$ nA
- (B) $10^{35}$ cm$^{-2}$ s$^{-1}$
- (C) Dilution factor $f < 50\%$ (.3 for ND$_3$)
- (D) 5 T and 1 K
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 (ND₃) Target
- Three Magnetic substates (+1,0,-1)
- Two Transitions (+1 → 0) and (0 → -1)
- Deuterons electric quadrupole moment \( eQ \)
- Interacts with electric field gradients within lattice
NRM Lineshape

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

\[-2 \leq R < 1\]

\[ R = \frac{\omega - \omega_d}{3\omega_q} \]

- \( \theta \) polar angle between the D bond and \( B_0 \)
- \( \phi \) azimuthal angle \( V_{ij} \) not symmetric
- \( \eta \) symmetry parameter (peak position)

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

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

\[ -2 \leq R \leq 2 \]

\[ \Delta E_+ = E_0 - E_1 \text{ with intensity } I_+ \]

\[ \Delta E_- = E_1 - E_0 \text{ with intensity } I_- \]
Homogeneous Broadening

- 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

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

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

\[ F = \frac{1}{2\pi x} \left[ 2 \cos(\alpha/2) \left( \arctan \left( \frac{\mathcal{Y}^2 - x^2}{2\mathcal{Y} x \sin(\alpha/2)} \right) + \frac{\pi}{2} \right) ight. \\
\left. + \sin(\alpha/2) \ln \left( \frac{\mathcal{Y}^2 + x^2 + 2\mathcal{Y} x \cos(\alpha/2)}{\mathcal{Y}^2 + x^2 - 2\mathcal{Y} x \cos(\alpha/2)} \right) \right] \]

\[ \mathcal{X}^2 = \sqrt{\Gamma^2 + (1 - \epsilon \hat{R} - \eta \cos 2\phi)^2} \quad \mathcal{Y} = \sqrt{3 - \eta \cos 2\phi} \]

\[ \cos \alpha = \frac{(1 - \epsilon \hat{R} - \eta \cos 2\phi)}{\mathcal{X}^2} \quad \epsilon = \pm 1 \]

fit to ND$_3$

\[ \eta \cos 2\phi \sim 0.04 \]

\[ \Gamma \sim 0.05 \]
Measurement of DMR Signal

- 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.

\[
P_n = \frac{2\hbar}{g^2 \mu_N^2 \pi N} \int_{-\infty}^{\infty} \frac{3\omega_Q \omega_D}{3R\omega_Q + \omega_D} \chi''(R) dR
\]

\[
= \frac{1}{C_E} \int_{-\infty}^{\infty} I_+(R) + I_-(R) dR,
\]

\[
Q_n = \frac{(I_+ - I_-)}{C_E}
\]

\[
Q_n = 2 - \sqrt{4 - 3P_n^2}
\]
Measurement of DMR Signal

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.

\[
\begin{align*}
n_+ & \approx N e^{\beta \hbar \omega_q} \left( 1 + \frac{2}{3} (\beta \hbar \omega_q)^2 \right), \\
n_- & \approx N e^{-\beta \hbar \omega_q} \left( 1 + \frac{2}{3} (\beta \hbar \omega_q)^2 \right), \\
n_0 & \approx N \left( 1 + \frac{8}{3} (\beta \hbar \omega_q)^2 \right), \\

P_n & = \frac{n_+ - n_-}{n_+ + n_- + n_0} = \frac{r^2 - 1}{r^2 + r + 1} + 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} + O((\beta \hbar \omega_q)^2)
\end{align*}
\]

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


A line-shape analysis for spin-1 NMR signals

The Spin Muon Collaboration (SMC)
Establish Calibration

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

Fig. 7. An enhanced signal of 44% polarization (circles) with the fitted curve superimposed (line).
• RF irradiation at the Larmor frequency induces transitions between $m=0$ and other energy levels

• RF induced transitions at a single $\theta$ 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

- 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

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

\[ \Delta P_{zz} = -3 \Delta P_z \]

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

Fig. 5. Some NMR spectra are shown for the procedure in which the pedestal of the (1 \( \rightarrow \) 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.
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 form of a Voigt
- Changes clearly at $R$ and -$R$ and that's 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

- 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
- Distortions to the lineshape in the form of Voigt
- Changes clearly at $R$ and $-R$ and that’s it
- Spectral diffusion seen but only at RF location during recovery
Bulk Behavior from Data into MC

- 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 $R$

- Distortions to the lineshape in the form of Voigt
- Changes clearly at $R$ and $-R$ and thats it
- Spectral diffusion seen but only at RF location during recovery
Bulk Behavior from Data into MC

- Distortions to the lineshape in the form of Voigt
- Changes clearly at $R$ and -$R$ and that's 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 \( r(R) = \frac{I_+(R)}{I_-(R)} \) for all possible intensities
- Generate a lineshape and model from results
- Improve as needed
Find Overlapping Ratio at $R$


$$2T_1 e \frac{d\rho_i}{dt} = \sum_{j \neq i} (\rho_j \omega_{ji} - \rho_i \omega_{ij})$$

\[ \rho^1(B_\mu, B_\nu) = \xi \omega_1 (\rho^2 - \rho^1) \]
\[ \rho^2(B_\mu, B_\nu) = \beta \omega_1 (\rho^4 - \rho^2) + \xi \omega_1 (\rho^3 - 2\rho^2 + \rho^1) \]
\[ \rho^3(B_\mu, B_\nu) = \beta \omega_1 (\rho^5 - \rho^3) + \xi \omega_1 (\rho^2 - \rho^3) \]
\[ \rho^4(B_\mu, B_\nu) = \beta \omega_1 (\rho^2 - \rho^4) + \xi \omega_1 (\rho^5 - \rho^4) \]
\[ \rho^5(B_\mu, B_\nu) = \beta \omega_1 (\rho^3 - \rho^5) + \xi \omega_1 (\rho^4 - 2\rho^5 + \rho^6) \]
\[ \rho^6(B_\mu, B_\nu) = \xi \omega_1 (\rho^5 - \rho^6). \]
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 $R$

\[ \begin{align*}
\dot{\rho}_1(B_v, R) &= \xi \omega_1 (\rho_2(R) - \rho_1(R)) \\
\dot{\rho}_2(B_v, R) &= \xi \omega_1 (\rho_1(R) - \rho_2(R)) \\
\dot{\rho}_3(B_v, R) &= 0 \\
\dot{\rho}_4(B_v, R) &= \xi \omega_1 (\rho_5(R) - \rho_4(R)) \\
\dot{\rho}_5(B_v, R) &= \xi \omega_1 (\rho_4(R) - \rho_5(R)) \\
\dot{\rho}_6(B_v, R) &= 0.
\end{align*} \]
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

- 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.

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 $-R$. 

![Graph showing Tensor Enhancement Mechanism for single position](image)
Tensor polarization in the line

Full target vector polarization of ~40%

- 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 $r(R)$

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

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

Examples for initial vector polarization 42%
Polarization Mechanism Sensitivity

\[ \Delta I = I(R) - I'(R) \]

- Preliminary look at Solid Effect and Differential Solid Effect
- Only slight variation in ratio leading to \(<0.4\%\) variation total area of at Optimized \(\Delta I\)
- Can be used in Monte Carlo and fitting constraint
MC Optimal Lineshape

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

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

Examples Optimized Tensor Polarization
Examples (1.3→5.4,13.6→23.8,52→58%)
Some Preliminary Comparison to Real NMR Data

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

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%)
Tests and Checks

- Specialized NMR studies to come (S-MAS) (hole-splitting)
- Lineshape vs Scattering polarization extraction $T_2$ 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