DNP @ UNH: Vector and Tensor Polarization Extraction from Line-Shape Analysis

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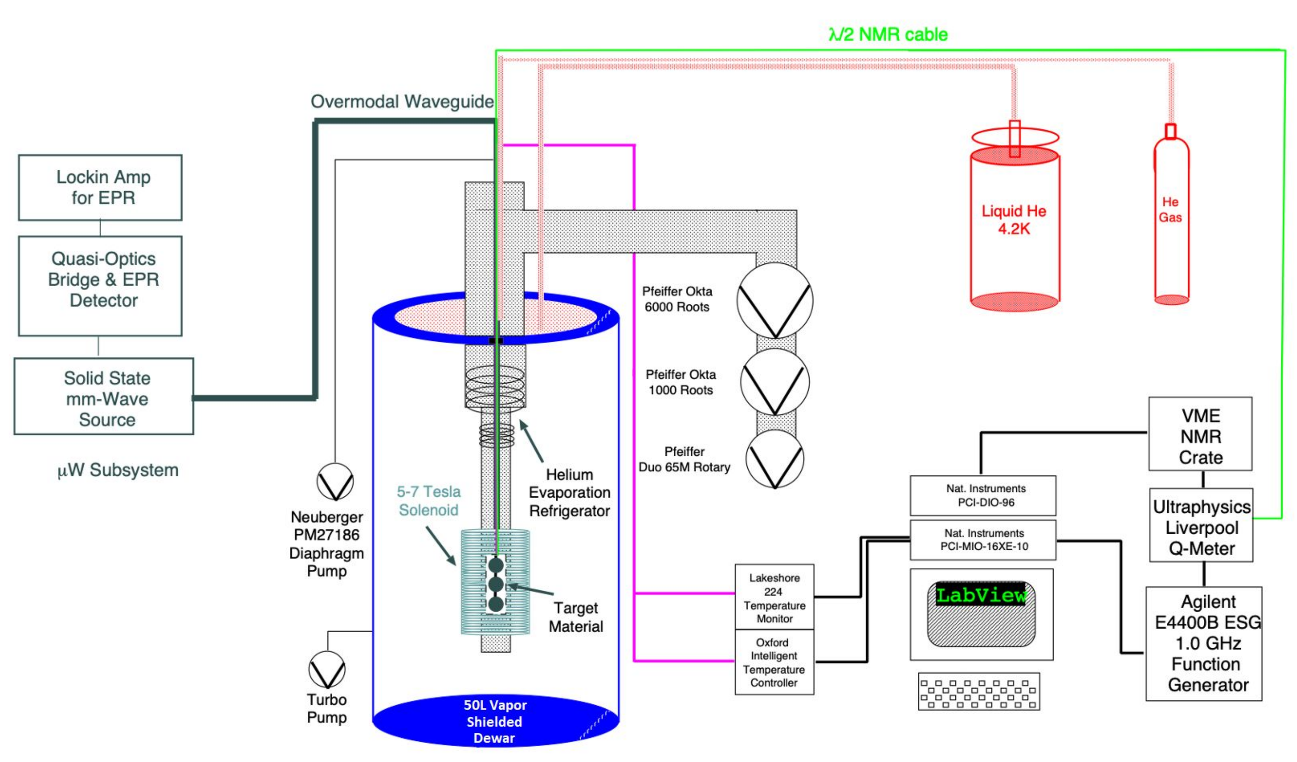
Background

The Solid Polarized Target group at UNH is developing a dynamically polarized target for use in measuring spin-structure and tensor spin observables including A_{zz}, T_{20} and b_1. These measurements can help distinguish between virtual nucleon and light cone nucleon-nucleon potentials; between "hard" and "soft" deuteron wave functions; and may provide an unambiguous signal for the detection of hidden color. Our lab has been successful dynamically polarizing deuterated targets such as chemically doped polymers and alcohols. Our next goal is to enhance tensor polarization to ~35%, including in deuterated ammonia.

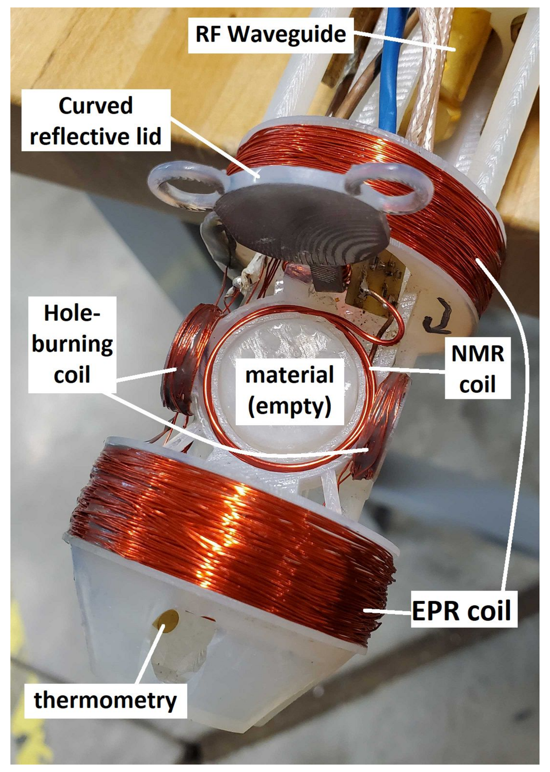
E. Long et al., C-12-15-005 PAC 44 (2016)

Lab Setup

- 5-7 T superconducting solenoid electromagnet
- Polarization monitored by LANL VME-based NMR system
  - P. McGaughey, et al., NIM A 995, 165045 (2021)
- 1K LHe Evaporation Fridge designed and maintained in-house
- Novel solid state mm-wave system
  - Only lab currently using such a system for nuclear physics targets!
- 3D printers - rapid prototyping/testing of parts
  - Examples: Target ladder, material capsules
  - Printed components survive 1K cryocycling & high radiation exposure



Lab schematic, drafted by Karl Slifer.

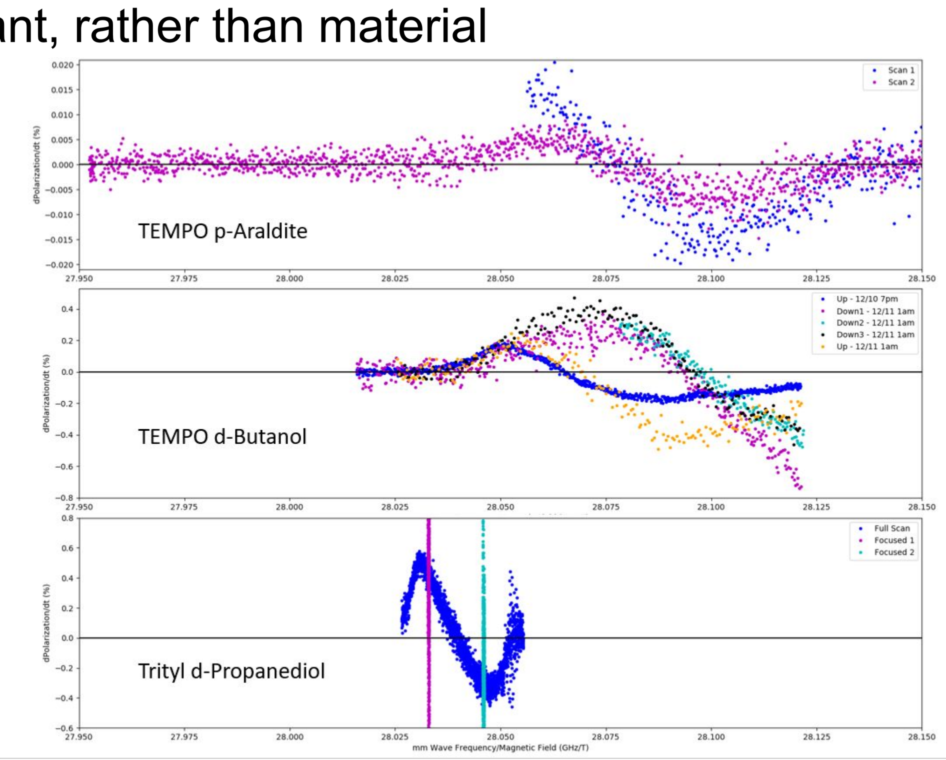


Polarized target cup in 3D-printed target ladder.

Members of UNH DNP inserting target into magnet.

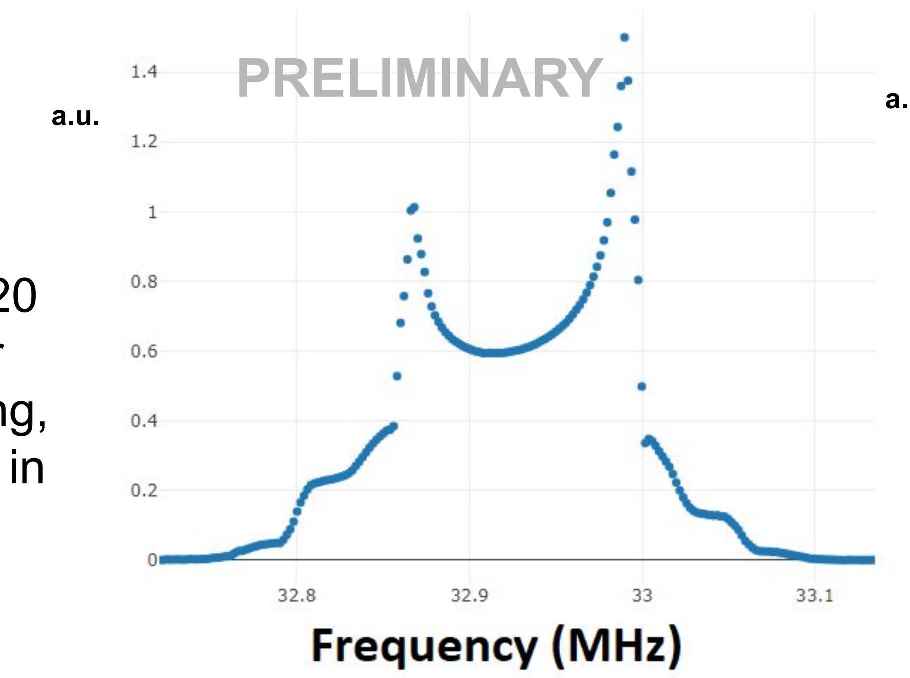
EPR Testing

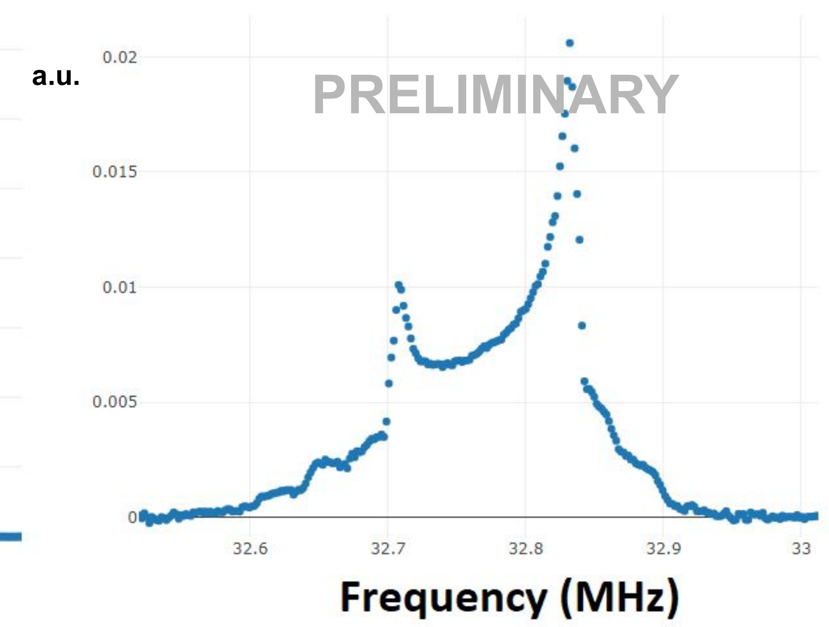
- Initial results indicate EPR linewidth is dependent on dopant, rather than material



Deuteron Signals

- 9/10/20: First deuteron signal
  - Chemically doped polymer
  - DNP enhanced P_z > 30%
- Deuteron signal observed again 12/20, 10/21, 12/21, 5/22
- Hole-burning first attempted 12/20
- 5/22: Demonstrated initial tensor enhancement via RF hole-burning, with current system optimization in progress





Future Plans

- Goal: Reach P_{zz} > 35%. Possible methods:
  - Add rotation mechanism to turn material during enhancement
  - Continue with hole-burning
  - Use EPR to pinpoint RF enhancement frequencies
- Goal: Polarize deuterated ammonia
- Goal: Incorporate hole-burning into curve-fitting method
- Continue with polarization simulations:
  - Can component spin-flip signals be separated in frequency?
  - Reduce signal width by manipulating quadrupole angles in material

Fitting Deuteron Signals

- Per Dulya, et al., deuteron NMR signal has the following functional form:

R, A, η, ϕ — compacting variables

$$\rho^2 = \sqrt{A^2 + [1 - \epsilon R - \eta cos(2\phi)]^2} \qquad R = \frac{\omega - \omega_d}{3\omega_q}$$

$$cos(\alpha) = \frac{1 - \epsilon R - \eta cos(2\phi)}{\rho^2} \qquad -3 \le R \le 3$$

functional form of signal

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

$\epsilon = \pm 1$

phi average

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

positive & negative spin flips

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

$$\theta = \omega_q/\omega_d$$

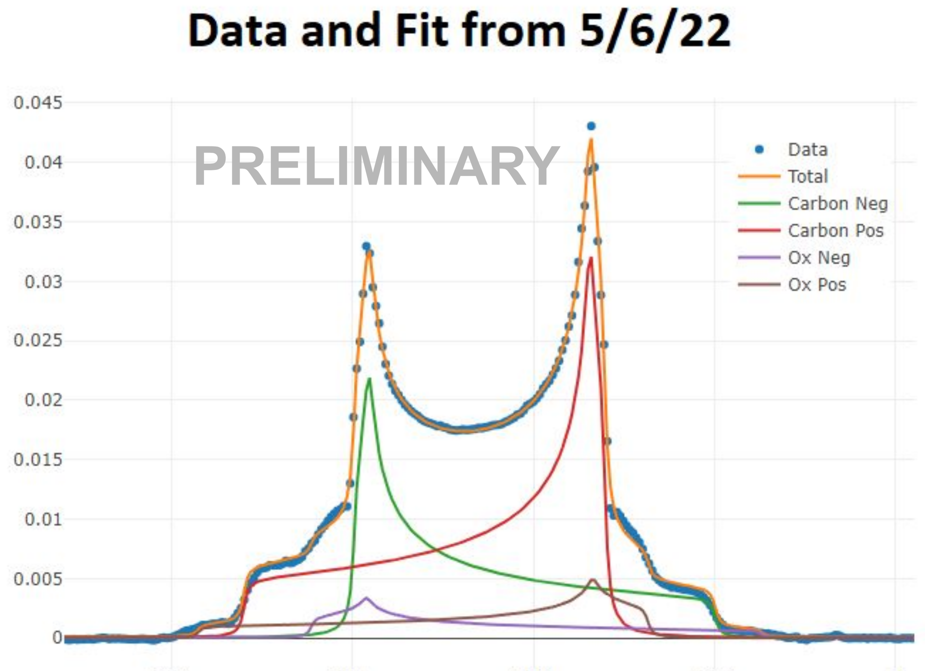
polarization

$$P_z = \frac{r^2 - 1}{r + r^2 + 1} \quad \text{or} \quad P_{zz} = \frac{r^2 - 2r + 1}{r^2 + r + 1}$$

Drawing on: C. Dulya et al., Nuclear Instruments and Methods in Physics Research A 398 (1997)

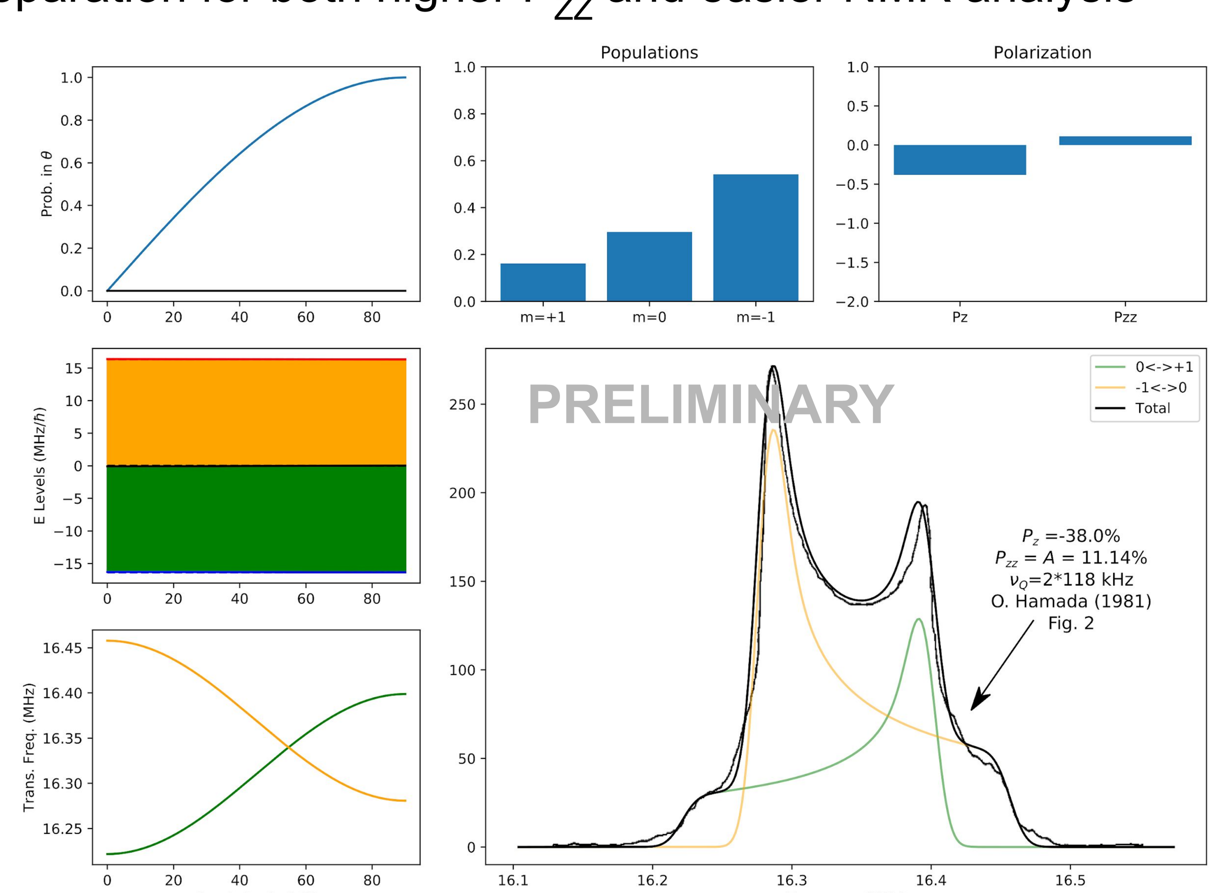
- Use curve fitting to solve for parameters:
  - ω_D - central frequency; ω_Q - frequency width; A - peak width; η - bond asymmetry; r - polarization asymmetry
- r is then used to determine P_z and P_{zz}
- For multi-bond materials like butanol, use K - ratio between O and C bonds

Data and Fit from 5/6/22



NMR Simulations

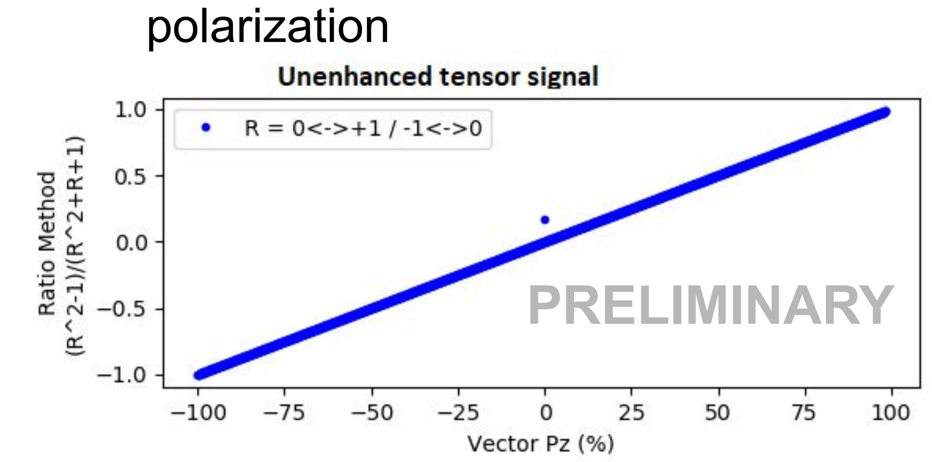
- Python simulation developed to see how to get P_{zz} from NMR signal
- Found deuteron signal shapes dependent on quadrupole angle population
- As angle function changes, peak separation changes - try to increase separation for both higher P_{zz} and easier NMR analysis

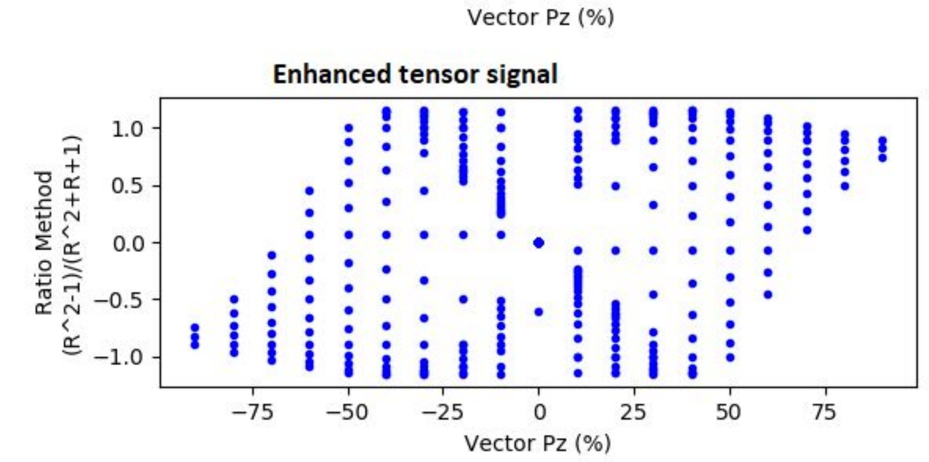


- Ratio method only applies when:

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

- Ratio method fails for arbitrary tensor polarization





Plots by Elena Long, drawing on:
- M. H. Cohen et al., Solid State Physics 5, 321 (1957)
- K Guckelsberger and F. Udo, NIM 137 (1976)

Acknowledgements

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