Automated Microwave Frequency Control in Dynamic Nuclear Polarization Experiments

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Introduction

- UVa Polarized Targets; Jlab, Fermilab
- Electron beam polarized target experiments
- Aim to create a controller capable of seeking/maintaining ideal frequency for polarization
- Increase the figure of merit (FOM) of DNP experiments

 $FOM = n_t \cdot f^2 \cdot P^2$

- $n_t = target \ thickness$
- f = dilution factor
- P = polarization measured over time

P ↑, FOM ↑





Dynamic Nuclear Polarization (DNP)

- Polarization: Alignment of the spin of particles in a given direction (typically $\overrightarrow{B_o}$)
- DNP: Transfer of electron spin polarization to the nucleus
- Described by Solid Effect
- Additional electrons are added when material doped with beam irradiation
- Signal picked up through NMR coil









.6 Image: Maxwell, J.(2011). Probing Proton Spin Structure: A Measurement of - at Four- Momenentum Transfer of 2 to 6 GeV2. Retrieved from http://libra.virginia.edu/catalog/libra-oa:5202







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Microwave Frequency

- Dictated by difference in nuclear Larmor and electron paramagnetic resonance frequencies (EPR)
- [140.0 GHz 140.4 GHz for NH₃ @ 5T] / [69.7 GHz 70.1 GHz @ 2.5 T] for positive polarization
- [140.4 GHz 140.8 GHz for NH₃ @ 5T] / [70.1 GHz 70.5 GHz @ 2.5 T] for negative polarization



"Frequency Drift"

- Optimal frequency for positive and negative polarization is *not* constant
- Changes take place as more centers are created in the material as a result of irradiation.
- Steady state of polarization at a particular frequency also vulnerable to other variables such as temperature, radiation damage, number of anneals, etc.



Image: Riechert, H. (1983). Polarization Properties of irradiated ammonia (NH3 and ND3) at 1K and 25 kG. AIP Conference Proceedings 95, 520 .

"Frequency Drift"



Image: https://www.jlab.org/Hall-C/talks/01_22_10/maxwell.pdf

Optimal Negative µWave Frequency vs Dose Since Last Anneal

140.56 r

Maintaining Highest Polarization

- Manually maintaining optimal polarization is tedious, error prone
- If characteristics of polarization growth/decay are understood, process can be automated
 - Input = EIO voltage divider value $\propto \mu$ -wave frequency
 - Output = Polarization value from NMR analysis software



Types of Motors

- Two motor types used with EIO
- Continuous DC motor
 - Most common motor currently in use (standard)
 - Shaft rotates continually whenever a voltage is applied
 - Movements are not very precise
- Stepper motor
 - Applying voltage causes the motor to "step" by a couple degrees, and then stop
 - Allows for much more controlled movements
 - For continuous motion, a series of pulses is used

Standalone Controller (for standard motor)

- Built to replace traditional manual frequency adjustment
- Components
 - Standard 2U Rack-mount hardware
 - Parallax P8X32A microcontroller
 - PL2303 USB to RS232 TTL serial communication
 - Parallax 4x20 LCD display
 - L298N H-Bridge motor controller
- Features
 - Front-panel readout and user interface
 - Remote control support
 - Automatic and manual control of motor
 - Works with different EIOs via calibration
- Required for use with "traditional" motor







Software controller

For Polarized Drell-Yan experiment with Sea Quest (E1039)

- New hardware available from CPI: stepper motor and power supply
- Stepper motor: benefits over "traditional" motor
 - Much more precise bellows position control
 - Amount to move can be directly specified
 - Controlled directly through RS232 serial
 - EIO power supply is also controlled via serial
 - System control via LabVIEW
- New software controlled microwave power supply
 - Software controlled transmit/standby, power
 - Software controlled cathode, anode and filament voltages
 - Monitor cathode, anode and helix currents
 - System control via LabVIEW





Automation Control

- Must seek optimal microwave frequency
 - Uses real-time polarization
 - Change position or stay fixed
 - Switch between positive and negative
- Must perform well given external variations
 - Thermal fluctuations
 - Beam trips
 - Decay from beam irradiation
- Developed Monte Carlo for testing efficiency and optimization under all these dynamics

LabVIEW Controller





- Motion of the motor should be based on the rate of polarization increase
 - An increase in the rate implies that the motor is moving in the right direction; a decrease implies that the motor should return to a previous position
- Rates calculated using three (or more) data points (pairs of polarization and time values)
 - Calculate slope connecting adjacent data points, and then average rates:

$$rate = \frac{\frac{P_3 - P_2}{t_3 - t_2} + \frac{P_2 - P_1}{t_2 - t_1}}{2}$$

 Averaging the rates gives better results when the polarization experiences fluctuations (due to thermal effects)



Optimal vs Seeking Algorithm

- Efficiently automates the process of a person seeking the ideal frequency
- Accurately converges to ideal frequency relatively quickly (~5 minutes)
- Quick "ramp-ups" when starting from good frequency
- Plots below taken from a run of the LabVIEW stepper motor controller, interfacing with simulation
 - Results from standalone controller box should be similar (uses same seek algorithm)





Behavior of ramp-up and decays are based on Differential Solid Effect

- Model for spin ½ from Leifson and Jeffries, 1961
 - Set of coupled differential equations for nuclear (P_n) and electron (P_e) polarizations:

$$T_{1e}\frac{dP_n}{dt} = \left(-\frac{T_{1e}}{T_{1n}} - \frac{C\alpha}{2} - \frac{C\beta}{2}\right)P_n + \left(\frac{C\alpha}{2} + \frac{C\beta}{2}\right)P_e$$
$$T_{1e}\frac{dP_e}{dt} = \left(\frac{\alpha}{2} - \frac{\beta}{2}\right)P_n + \left(-1 - \frac{\alpha}{2} - \frac{\beta}{2}\right)P_e + P_0$$

- α and β are parameters corresponding to transitions (induced by microwave), α drives negative while β drives positive for given frequency
- *C* is the ratio of electrons to nuclei
- T_{1e} , T_{1n} , and P_0 are constants
- General 'reduced' solution is of the form $P_n(t) = A + Be^{-k_1t} + De^{-k_2t}$ 9/25/2016

Simulation

- Written in LabVIEW to work with stepper motor
 - Can also be run by itself to produce data
- Implements model
 - Parameters α and β calculated from frequency
 - Uses experimental fit to steady state P_n







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Single Exponential Approximation

- Fit experimental data to function of the form $P_n(t) = P_{\infty} + Ae^{-\lambda t}$
 - Full model contains two exponential terms, one of which is very small
 - Easier to analyze in this form





Growth/Decay Data – April and December "Cooldown"



Conclusion

- Two controller systems
 - Standalone controller box supports continuous DC motors (self contained MC)
 - LabVIEW controller supports stepper motors/power supply
 - Both systems offer automatic and manual control of polarization experiments
- Simulation combines theoretical model and experimental data
 - Determine α and β
 - Important to check the seeking algorithm
- Future plans
 - Implement the simulation for spin 1 system
 - Implement tools to control power supply
 - Develop time-independent seeking algorithm



Back up

Limitations

- Fairly slow process, especially when far off of f_{ideal}
- Time *dependent*: $\frac{d}{dt}(-e^{-t}) = e^{-t}$
- Frequently moves in wrong direction
 - Rate is *always* decreasing in exponential growth/decay







Time-independent Seek

- Seeking frequency by maximizing $|\lambda \cdot P_{\infty}|$ would eliminate time-dependence
 - Unlike the raw rate of polarization increase, this quantity does not depend on time
- To calculate λ requires the second derivative of $P_n(t)$:

$$P'_n(t) = -A\lambda e^{-\lambda t}$$

$$P''_n(t) = A\lambda^2 e^{-\lambda t}$$

$$\lambda = \frac{-P_n''(t)}{P_n'(t)}$$



- Works well under perfect conditions, but thermal fluctuations make $P_n''(t)$ very hard to calculate accurately
- Time-dependent seek actually behaves better when fluctuations are present



LabVIEW Controller

- Interfaces directly with motor over RS232
 - No need for standalone controller box
- Features
 - Automatic and manual control
 - Takes advantage of precise motor steps
 - Built-in experimental simulation for testing
 - Data output during automatic mode
 - Easy frequency calibration
- Works only with stepper motor

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