

Spin-Polarization using Microwave Induced Dynamic Nuclear Polarization

Polarized Sources, Targets, and Polarimetry Workshop 2019

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Polarized Target Overview

Microwave Generator

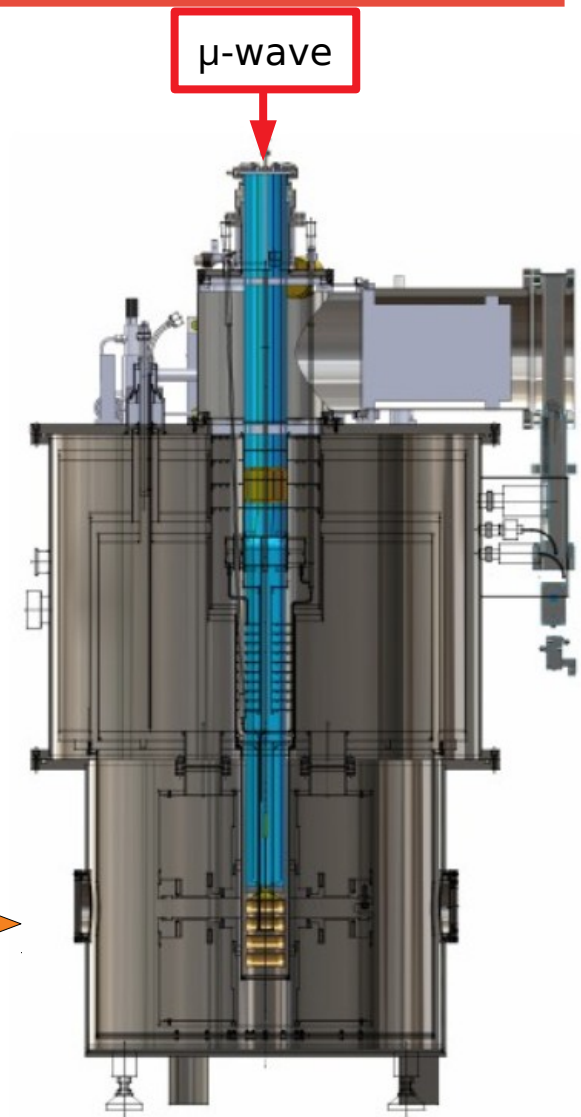
Microwave Controls System

Dynamic Nuclear Polarization Simulations

Automated Polarization Optimization

UVA microwave and polarized target system:

- 5T superconducting split coil magnet.
- 140 GHz microwave source.
- 8 cm long solid NH_3/ND_3 targets.
- $dB/B < 10^{-4}$ at 5T over 8 cm



Microwave Generator & Controls System

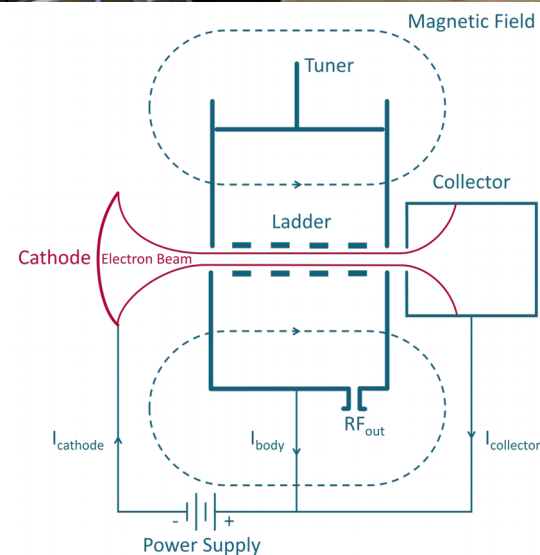
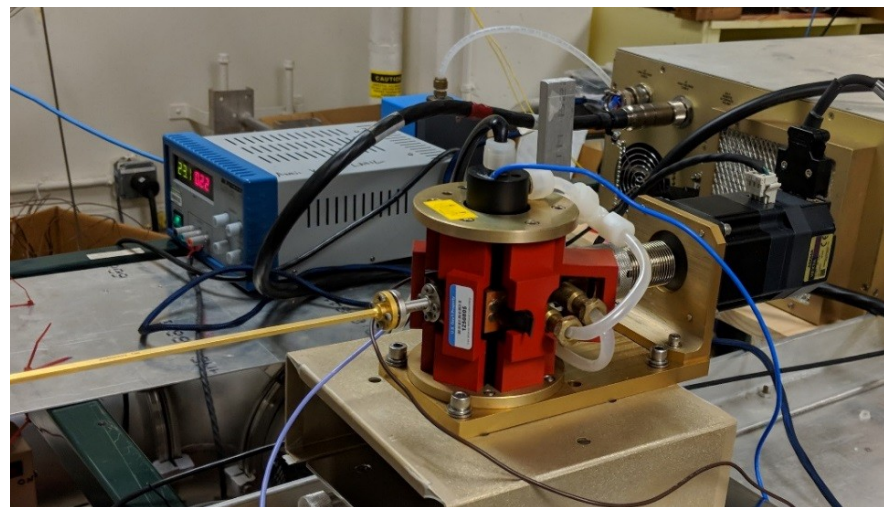
Microwave System

Variable frequency microwave system used to drive transitions in the DNP process → Extended Interaction Oscillator(EIO)

The EIO is coupled to target waves guides which send the microwaves through the target stick terminating at a gold plated copper horn trained on the target material cups.

Driving frequency defined by ESP, NMR, and magnetic field.

- EIO attenuated from 20W → 1W scale.
- 140 GHz (F→D wave) microwaves
- Cavity adjustment via stepper motor allows for 1.5% frequency adjustment.
- Voltage adjustment allows for another 0.5% adjustment.



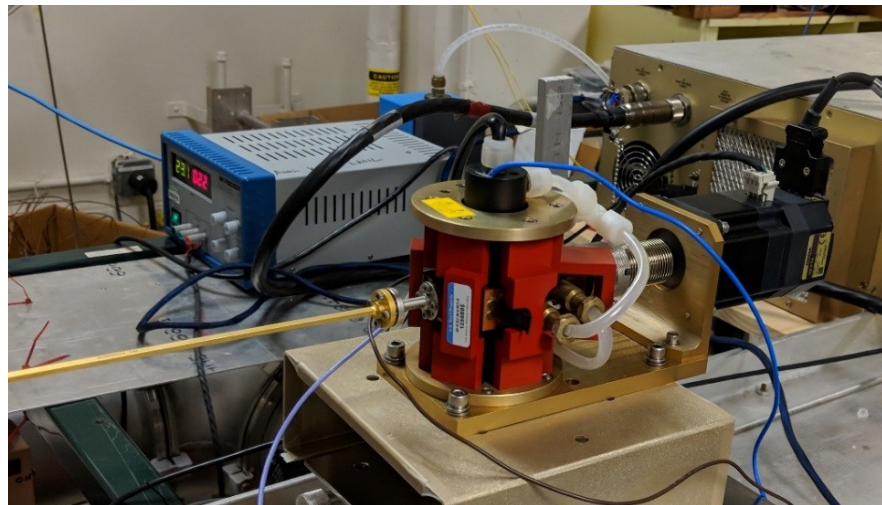
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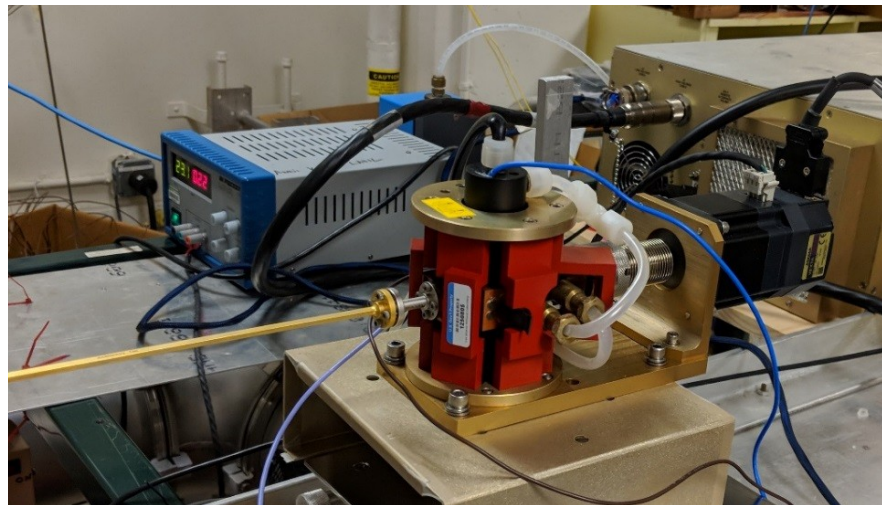
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Driving frequency defined by ESP, NMR, and magnetic field.

The microwave systems is cooled using an external chiller providing over 2kW of power dissipation; the microwave needs around 1kW total.

The outlet flow rate and water temperature are interlocked for safety.

The microwave frequency is read out via EIP 588C Frequency Counter.

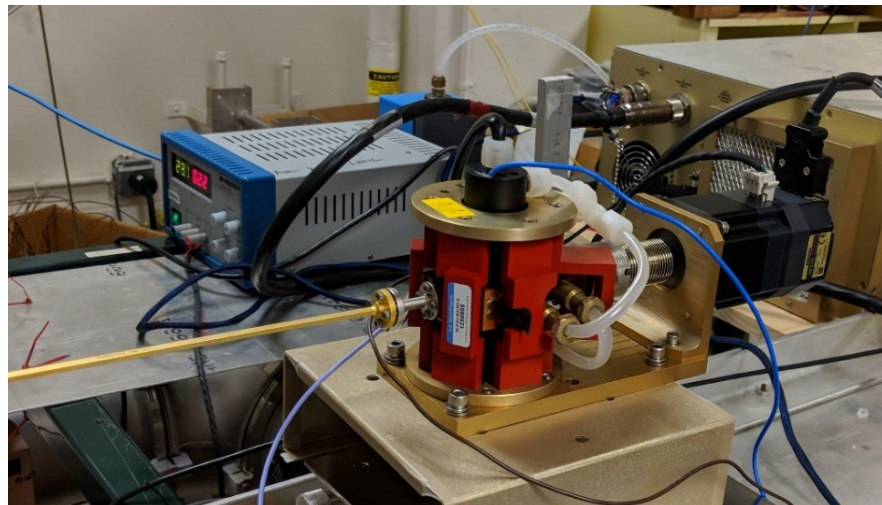


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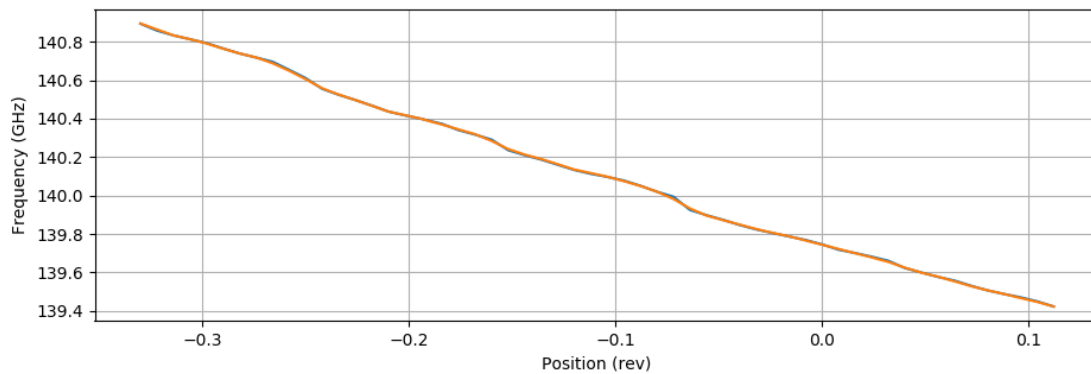
Driving frequency defined by ESP, NMR, and magnetic field.



In addition to being read out the frequency-position space so mapped to allow for frequency seeking.

Relationship is mostly linear, very much so locally.

Map used to extrapolate using nearest neighbors and return calculated frequency.

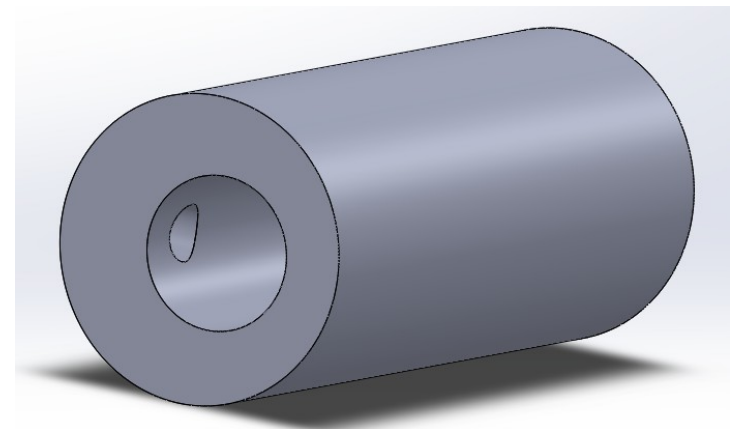
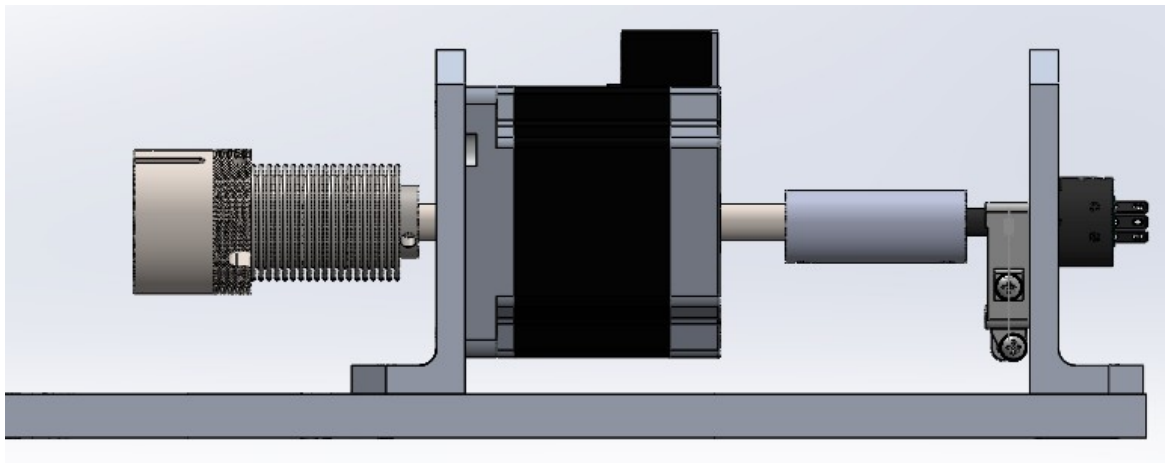
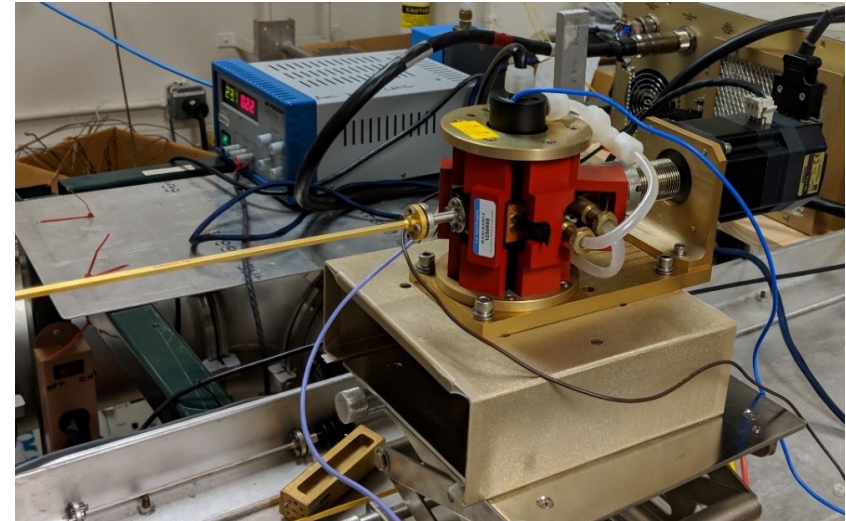


Microwave System

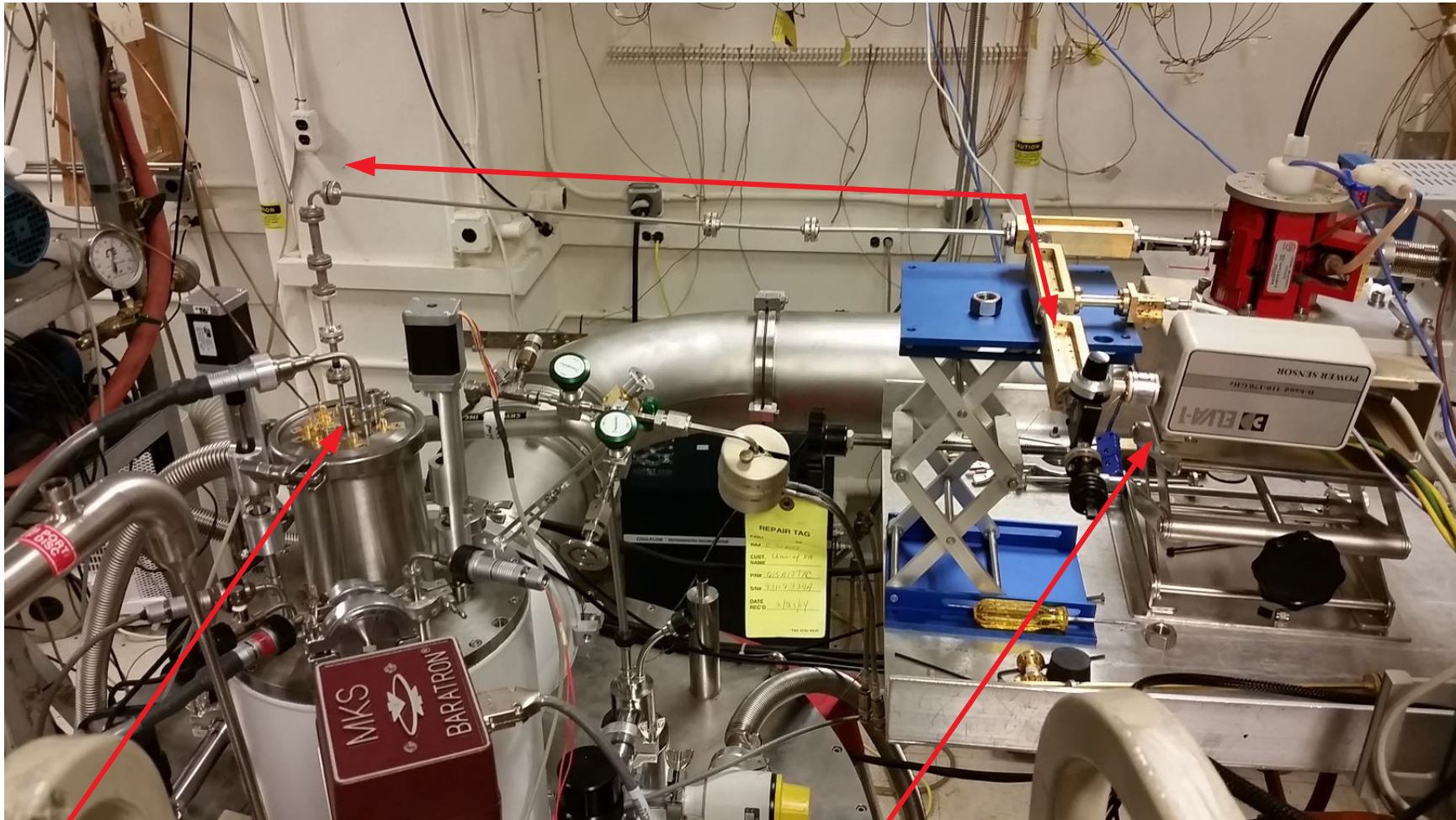
Microwave frequency set by cavity size attached to bellows on outside of EIO - the cavity size is adjusting by a stepper motor.

Original manufacturer motion system replaced to separate controller and driver from motor - needed for high radiation area.

System was redesigned to have a separated controls system adding limit sensors and absolute hardware position tracking.



Microwave System

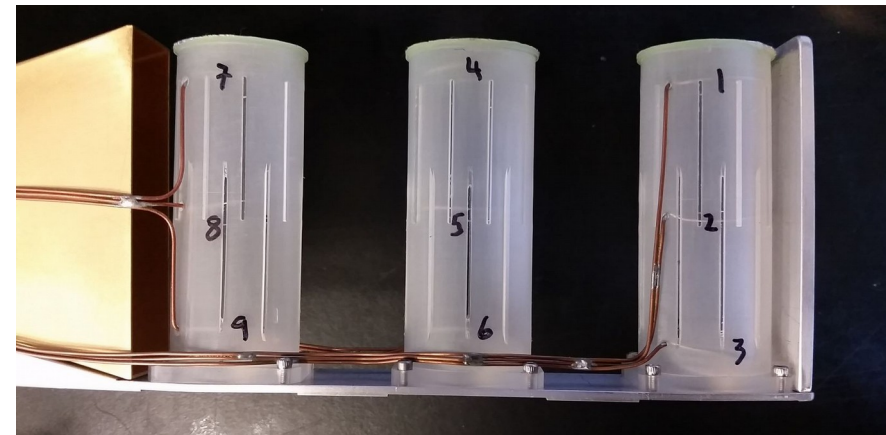
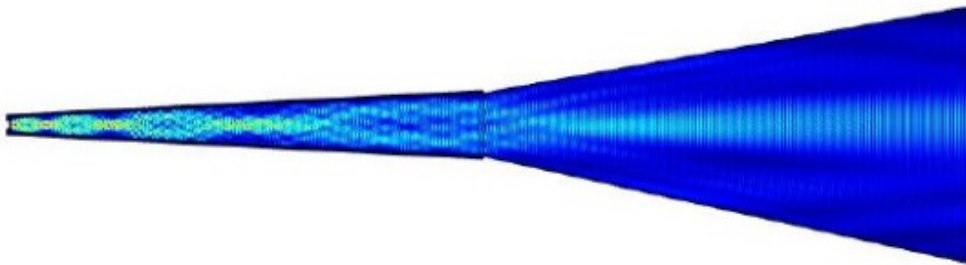


Target Stick

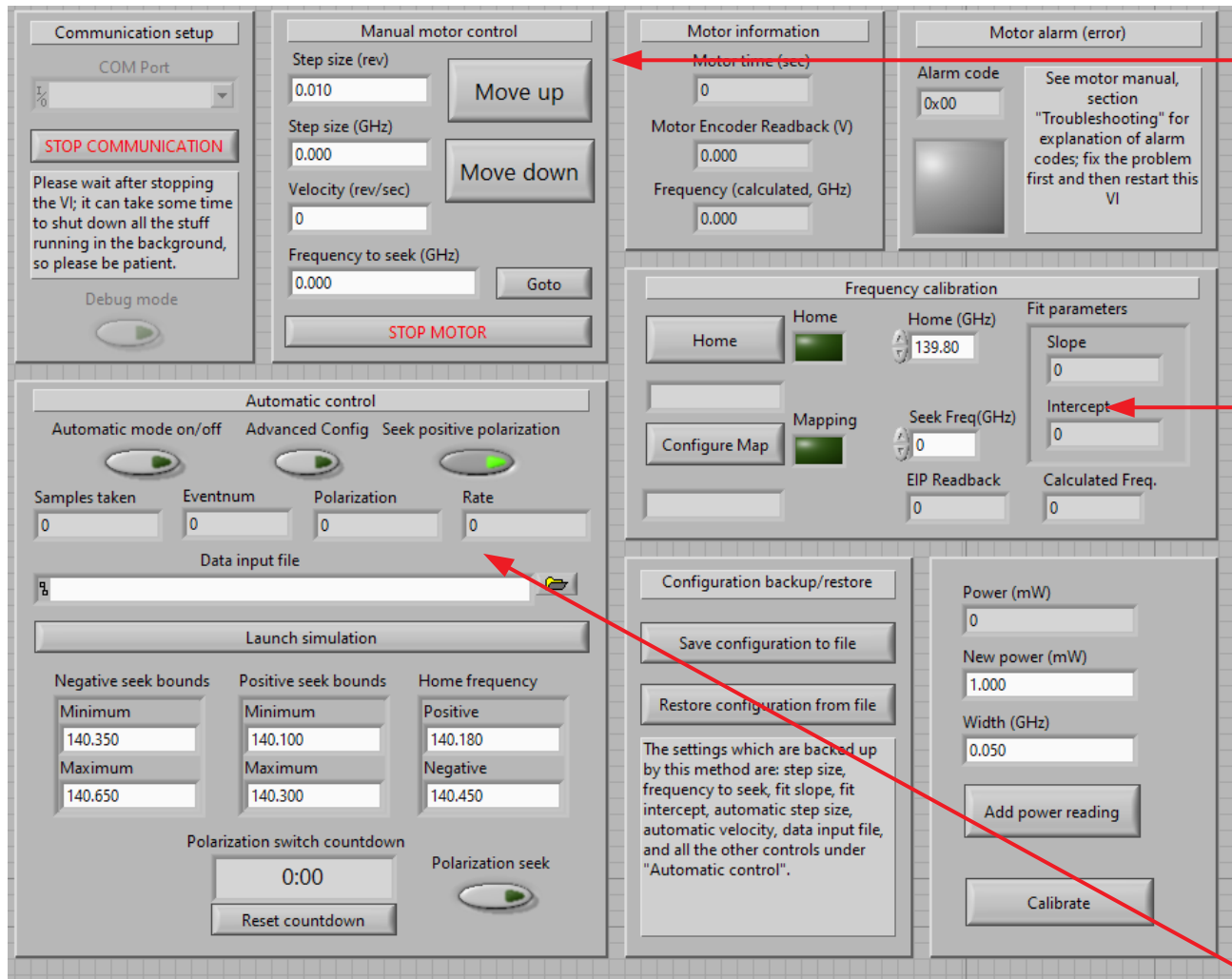
Power Meter

Target Inserts and Microwave Horn

- One proton insert with four target cups. As well as one deuteron insert with at three cold NMR coils per cup.
- Target inserts constructed of a carbon fiber shell for minimal thermal conductivity and guidance.
- Each insert has three thermal sensors to monitor the annealing plate temperatures.
- Three NMR coils installed on each target cup.



Target Controls Frontend



Manual motor controls

Frequency Calibration

Simulation and automation

DNP Simulations & Frequency Drift

Material Degradation and Frequency Shift

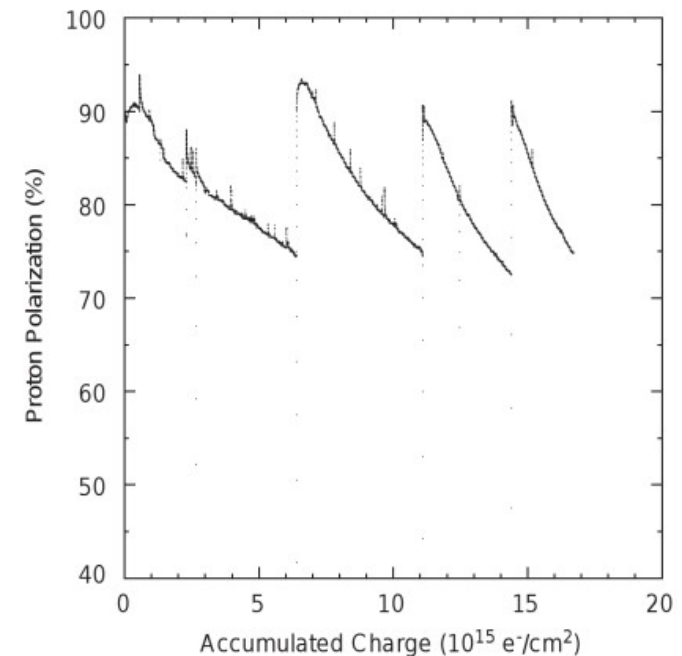
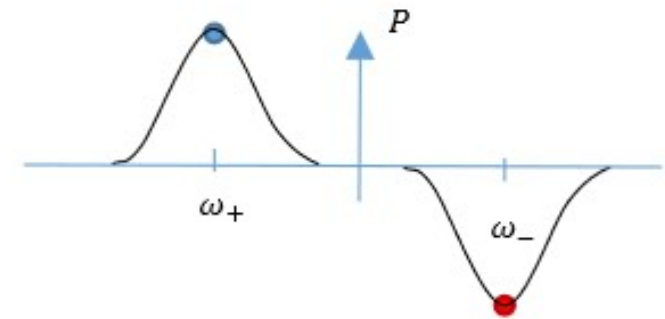
The frequency optimal for the DNP process is defined by the electron paramagnetic resonance and the nuclear Larmor frequencies.

- Positive polarization: 140.2 ± 0.2 GHz @ 5T
- Negative polarization: 140.6 ± 0.2 GHz @ 5T

The optimal frequency is not constant however and is influenced heavily by the degradation of color centers in the material.

This decreases nuclear relaxation time and widens the ESR line width.

Annealing can be used to promote recombination reactions and recover polarization but only a limited number of times.



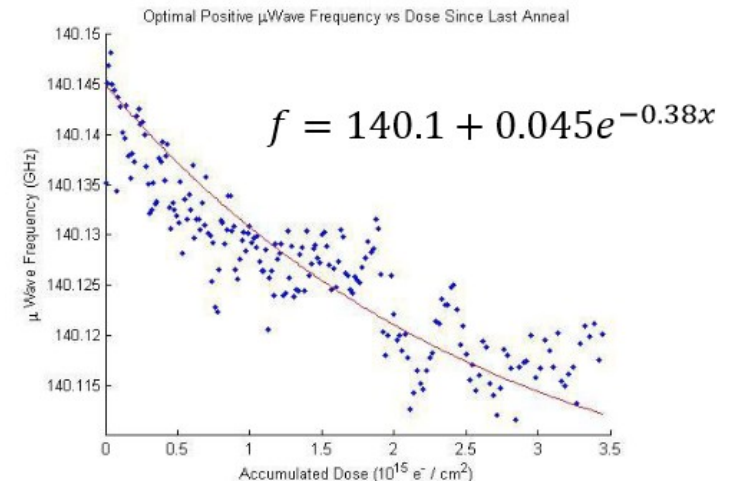
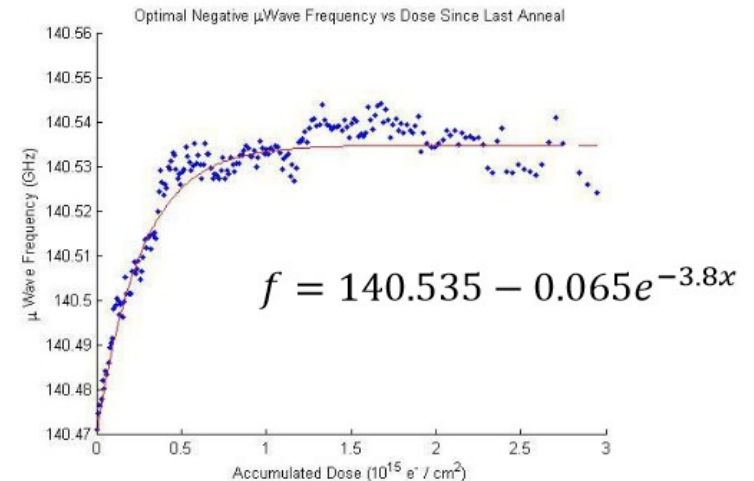
Frequency Drift

Steady-state polarization also sensitive to temperature, microwave power, and number of anneals.

Would like to maximize polarization between anneals by accounting for frequency shifts.

The frequency drift can be accounted for using manual controls but is error prone and not optimal.

An understanding of the growth(decay) behavior allows for automation of process.

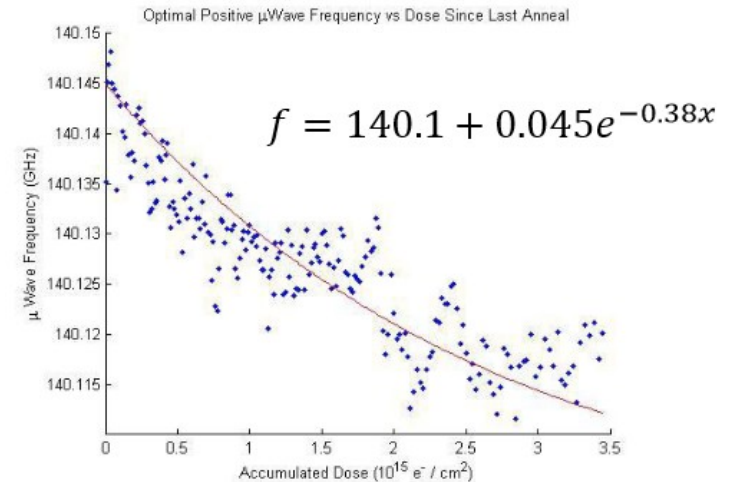
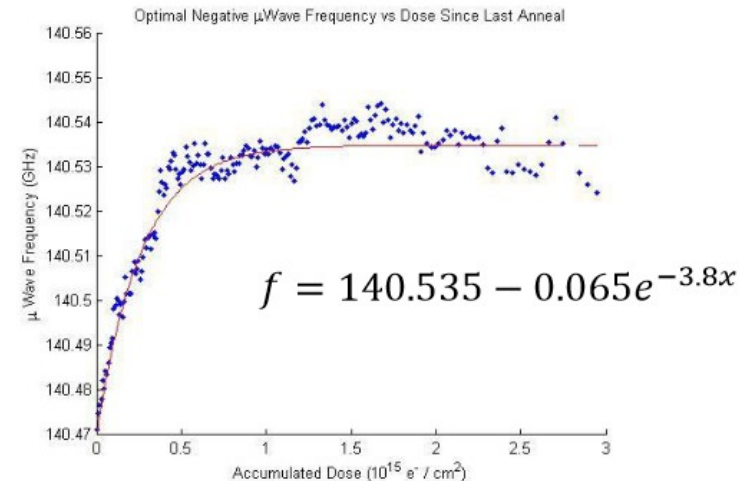


Automation Controls

System Requirements:

- Must actively seek optimal microwave frequency.
- Uses real-time polarization feedback.
- Switch between positive and negative.
- Must perform well given external variations thermal fluctuations, beam trips, material degradation, power fluctuations.

Need simulation to tune system to optimize algorithm for different materials, systems, and external factors.



Simulation of Solid State Effect

Model for spin-1/2 system based on Leifson and Jefferies, 1961.

Spin system describe by a set of coupled differential equations:

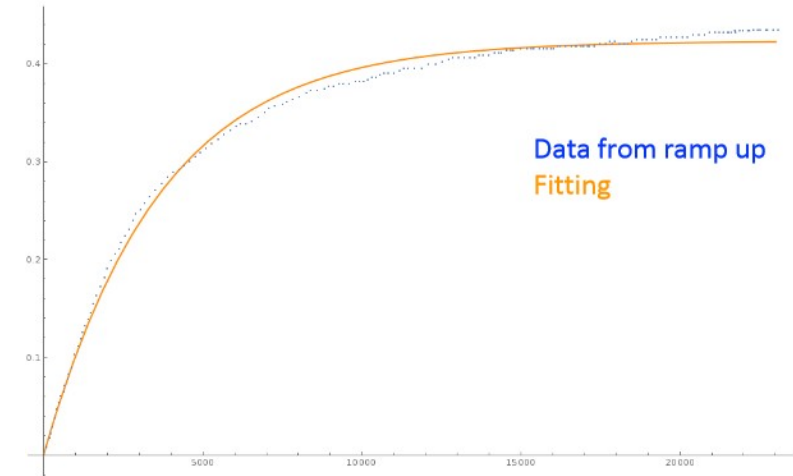
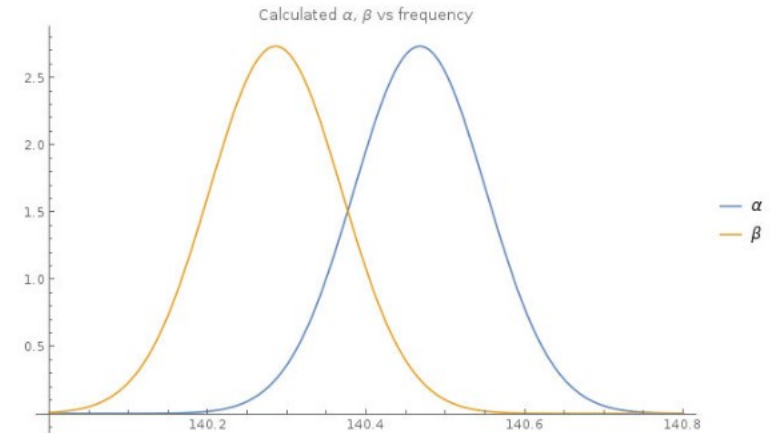
$$T_{1e} \frac{dP_n}{dt} = \left(-\frac{T_{1e}}{T_{1n}} - \frac{C\alpha}{2} - \frac{C\beta}{2} \right) P_n + \left(\frac{C\alpha}{2} + \frac{C\beta}{2} \right) P_e$$

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

Where α and beta β are related to the microwave induced transitions driving the negative (positive) polarization.

C is the ratio of electrons to nuclei in the sample.

T_{1e} and T_{1n} are the electronic and nuclear relaxations times respectively and P_0 is the equilibrium polarization.



Simulation of Solid State Effect

The reduced generalized solutions are of the form,

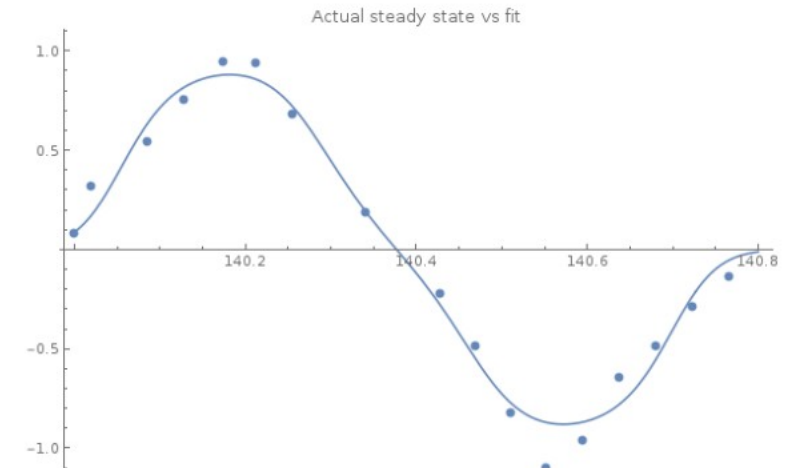
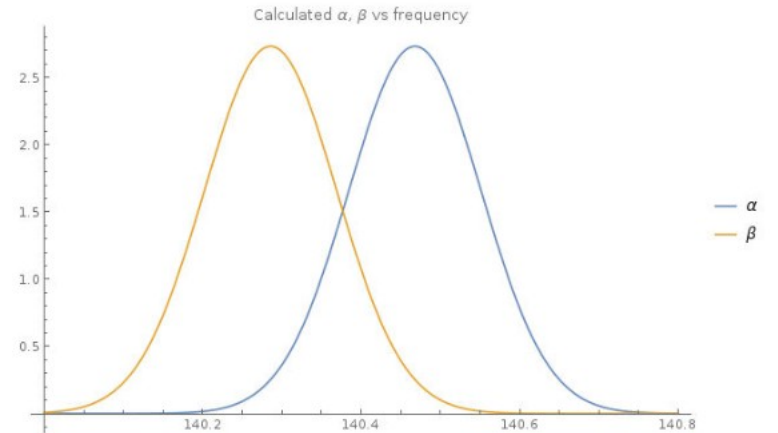
$$P_n(t) = A_0 + A_1 e^{-k_1 t} + A_2 e^{-k_2 t}$$

The steady-state nuclear polarization in terms of α and β is,

$$P_o = \frac{T_{1n} C (\beta - \alpha)}{T_{1e} (2\alpha + \beta) + T_{1n} (\alpha + \beta + 2\alpha\beta)}$$

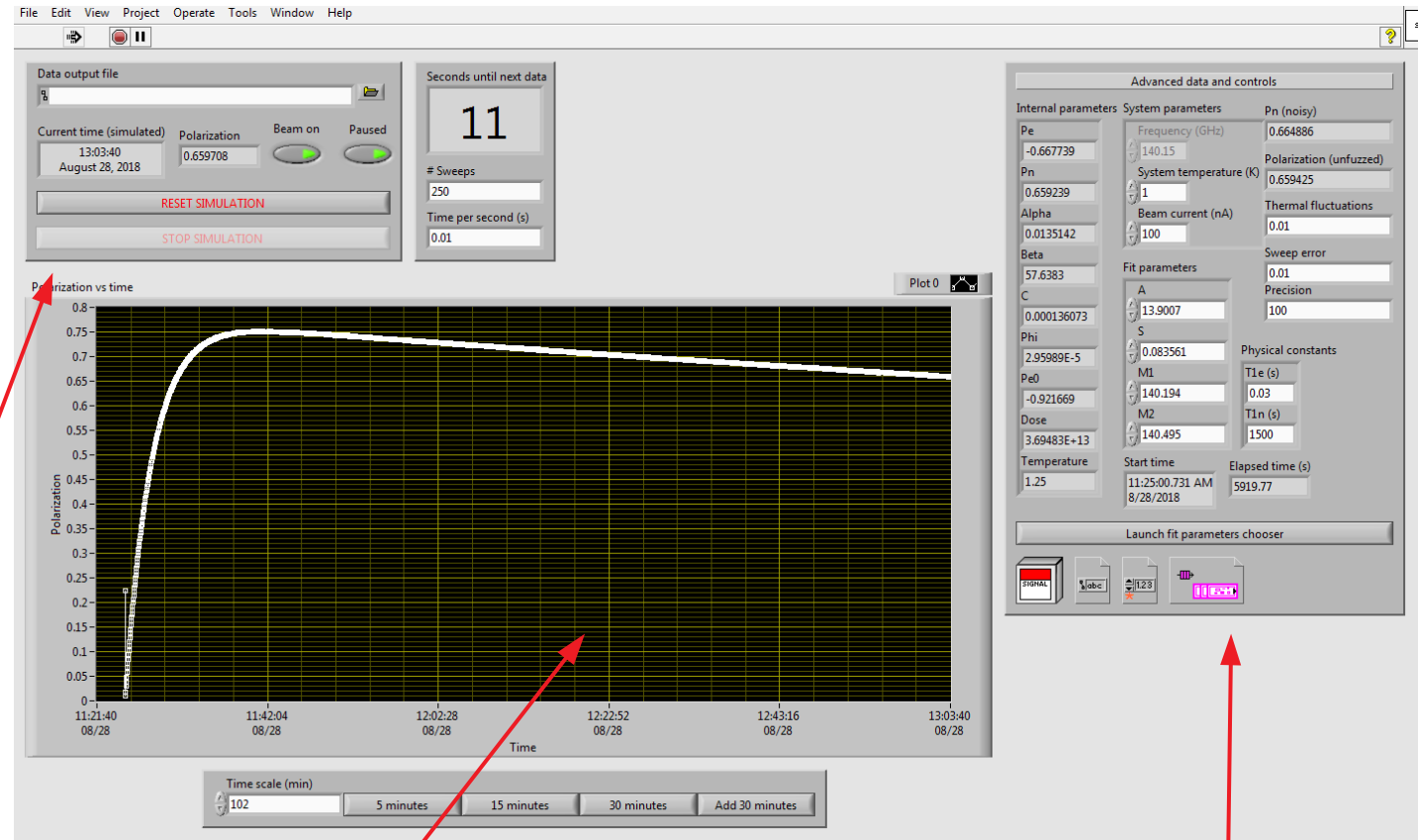
The frequency dependent model parameters $\alpha(f)$ and $\beta(f)$ are overlapping distributions driving the steady-state nuclear polarization.

The positive polarization is driven by $\beta(f)$ and the negative by $\alpha(f)$ and can be extracted from experimental data by fitting $P_n(t)$ over the frequency domain.



LABVIEW Simulation Controls

- The simulation was developed in Labview to compliment the current motor controls scheme.
- Simulated model data and polarization information written to output file.
- Advanced controls make simulation fully configurable.



Data Output

Simulated data

Advanced Configuration

LABVIEW Simulation Controls

The screenshot displays a LabVIEW simulation window with the following components:

- Alpha/beta distributions:** A graph showing two Gaussian curves. The blue curve (Alpha) is centered at approximately 140.3 GHz, and the red curve (Beta) is centered at approximately 140.5 GHz. The y-axis is labeled 'Alpha/beta' and ranges from 0 to 2.8. The x-axis is labeled 'Frequency (GHz)' and ranges from 140 to 141.
- Steady state distribution:** A graph showing a white curve representing the steady state distribution. The y-axis is labeled 'Steady state' and ranges from -1 to 1. The x-axis is labeled 'Frequency' and ranges from 140 to 141.
- Fit parameters:** A table of parameters for fitting the distributions.
- Physical constants:** A table of physical constants.
- Choose preset:** A dropdown menu showing 'ND-3' and buttons for 'Load from preset', 'Save as new preset', and 'Overwrite selected preset'.
- Internal controls:** A panel with icons for file operations and a 'SIGNAL' icon.
- Optimal frequency and steady state:** A table of optimal values for frequency and steady state.
- Explanation of fit parameters:** A text box explaining the parameters A, S, M1, and M2.

Fit parameters				Physical constants		
A	S	M1	M2	T1e (s)	T1n (s)	C
0.572086	0.0835606	140.286	140.486	0.03	1500	0.000136073

Optimal frequency (positive) (GHz)	Optimal steady state (positive)
140.214	0.742
Optimal frequency (negative) (GHz)	Optimal steady state (negative)
140.558	-0.742

Explanation of fit parameters:
The parameters A, S, M1, and M2 control the distribution of alpha and beta as shown above. The steady state distribution will be computed from these.
A: the height of the Gaussian distributions for alpha and beta
S: the standard deviation of the Gaussian distributions for alpha and beta
M1: the mean of the Gaussian distribution for beta
M2: the mean of the Gaussian distribution for alpha

Adjustable model parameters

Material Presets

Automated Polarization Optimization

Automated Polarization Algorithm

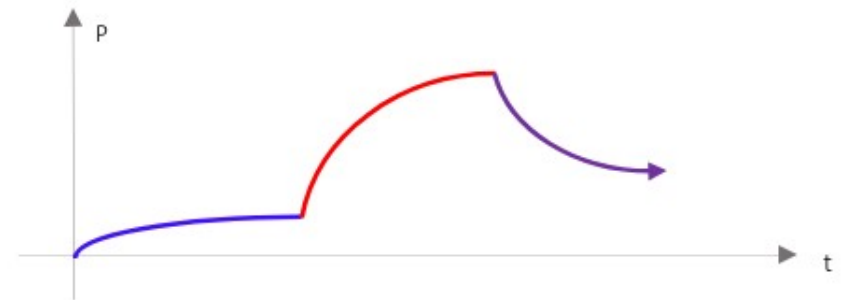
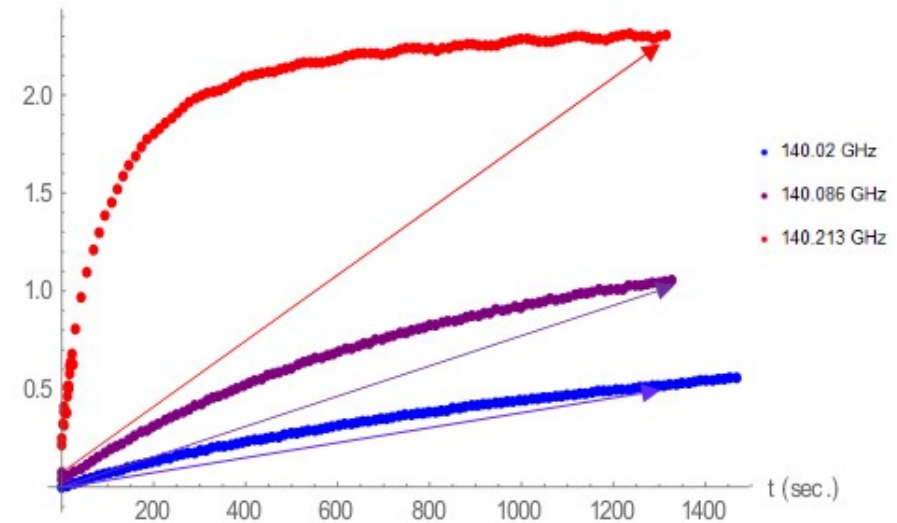
Remote control of the motor and frequency readback allows for a feedback loop to monitor and adjust the frequency based on the average polarization growth rate.

Increased growth → frequency adjustment in the correct direction.

Decreased growth → frequency adjustment in the wrong direction.

The average rate is calculated by sampling three or more data points to filter out small t fluctuations, ie. thermal noise.

$$\langle R \rangle = \frac{1}{2} \left(\frac{P_3 - P_2}{t_3 - t_2} + \frac{P_2 - P_1}{t_2 - t_1} \right)$$

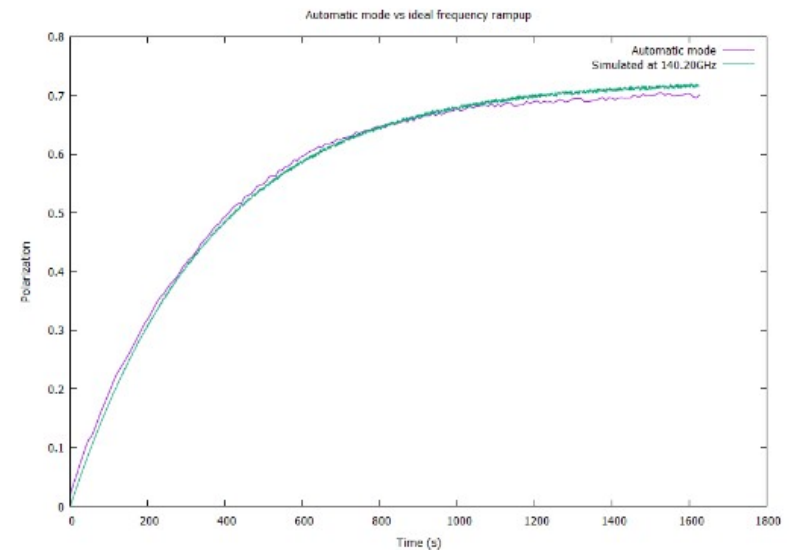
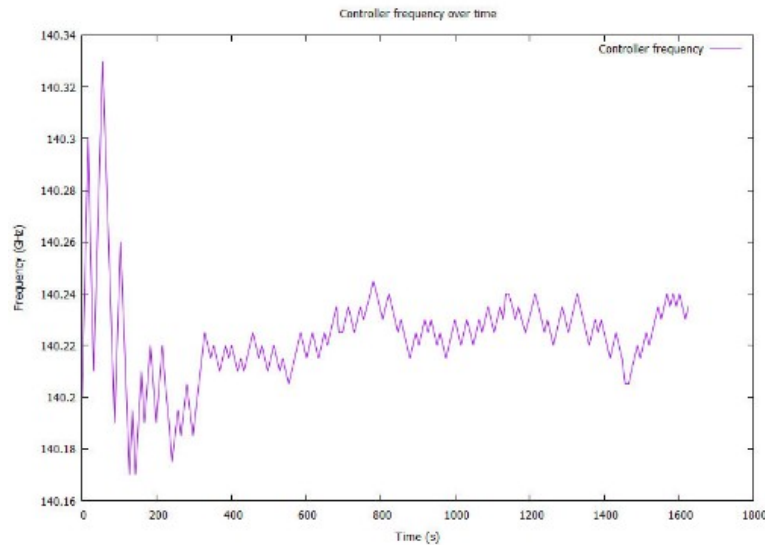


Feedback Adjustment on Simulation

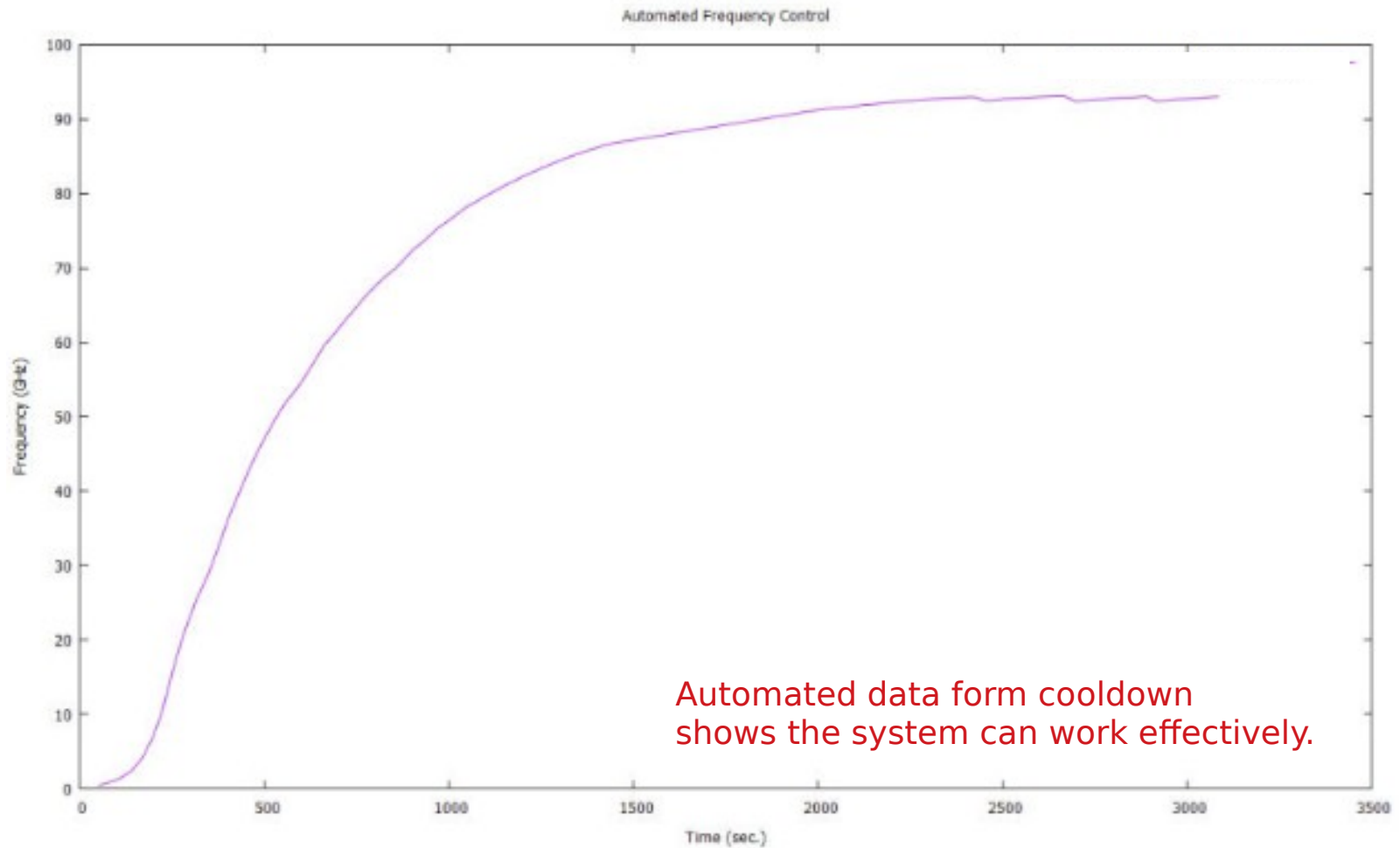
The automated polarization adjustment behaves efficiently matching the simulated growth rate.

Ramps up to optimal frequency relatively quickly if given a good initial condition.

In experimental running the polarization feedback given by NMR measurement.



Automated Control Results



Conclusion & Future Plans

- Microwave control system modified for high radiation environment.
- Rate equations provide good model to polarization growth in time as well as a good estimate of the optimal frequency for maximal polarization.
- Simulation provides good check of feedback algorithm.
- Simulations also useful in training target operators for upcoming experimental shifts.
- Feedback algorithm effective in optimization of polarization.

- Add simulation of spin-1 system.
- Modeling of beam related effects.

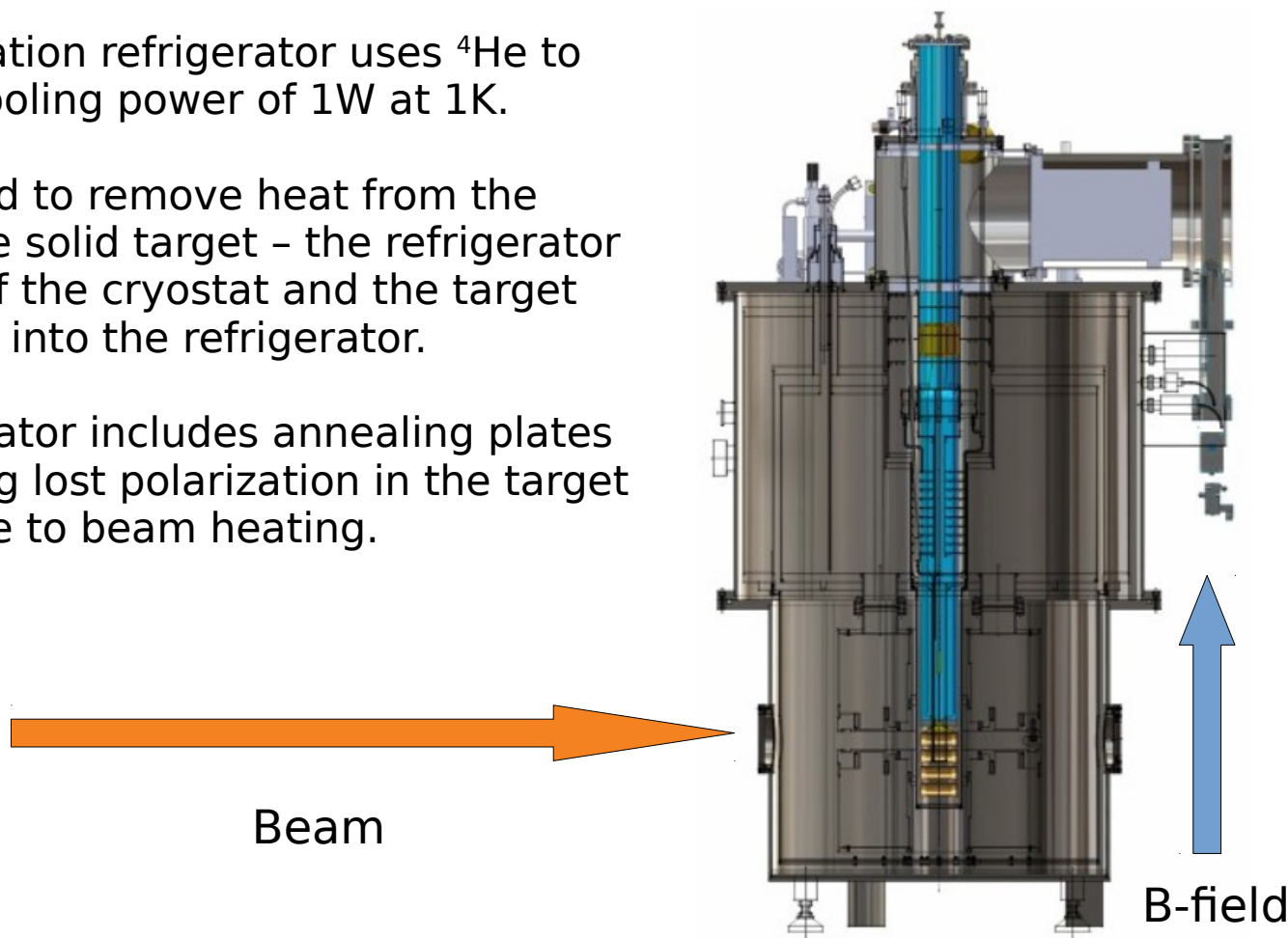
Thank You!

Target Cooling and Evaporation Refrigerator

The evaporation refrigerator uses ^4He to provide a cooling power of 1W at 1K.

Cooling need to remove heat from the beam on the solid target - the refrigerator sits inside of the cryostat and the target insert slides into the refrigerator.

The refrigerator includes annealing plates for retrieving lost polarization in the target material due to beam heating.



Spin Polarized Solid Targets

How do we obtain significant nucleon polarization?

The simplest way is via interaction with magnetic moment, μ . This is Zeeman splitting.

An ensemble of particles cooled and placed in an external B-field create $2J+1$ energy levels

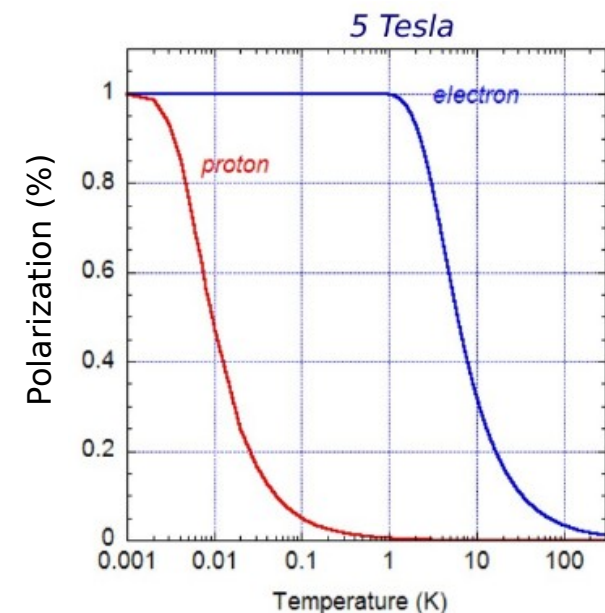
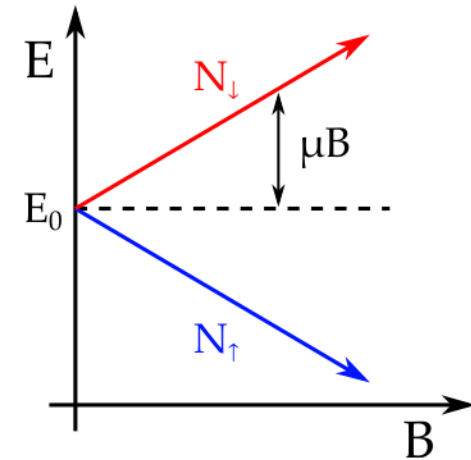
The vector polarization at thermal equilibrium is given to be:

$$P_{TE} = \frac{e^{\mu B/kT} - e^{-\mu B/kT}}{e^{\mu B/kT} + e^{-\mu B/kT}} = \tanh\left(\frac{\mu B}{kT}\right)$$

Brute Force: High B-field, Low T

- Simple and works for most any material.
- Requires high magnetic field
- Low temperatures \rightarrow low luminosity
- Takes a long time to polarize.

... but there is a better way!



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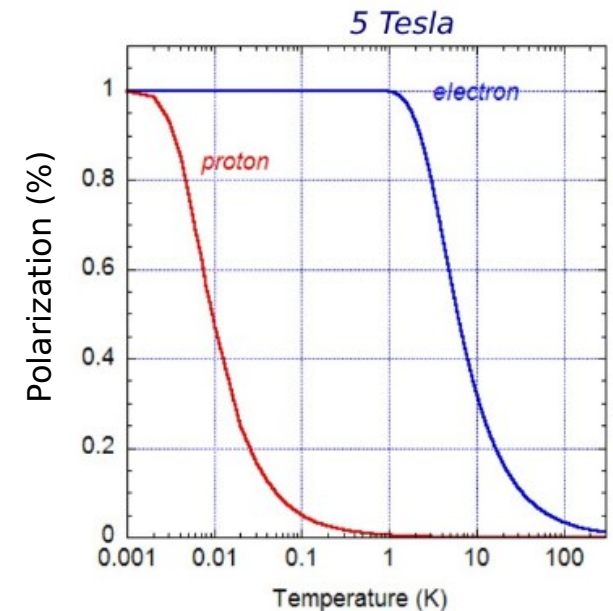
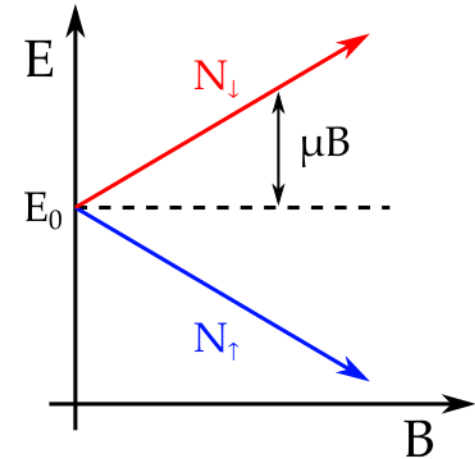
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Dynamic Nuclear Polarization: High B-field, Moderate T

- Use doped target materials with paramagnetic centers.
- Centers are polarized by external magnetic field.
- Use microwave to transfer polarization to the nucleon via pumping.
- The disparity in relaxation times between the electron (ms) and the nucleon (minutes \rightarrow hours) makes high spin polarization possible.



Dynamic Nuclear Polarization

For a system with of unpaired electrons in the target material, hyper-fine splitting gives four discrete energy levels.

$$H = \mu_e B + \mu_p B + H_{ss}$$

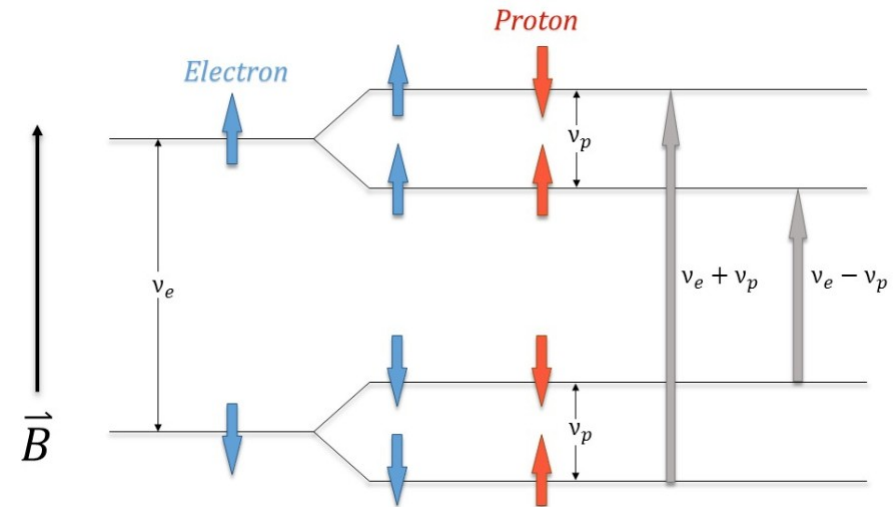
Applying an RF signal at the proper frequency we can drive the nucleons into a preferential state; the relatively short relaxation time of the electron versus the proton is crucial in pumping the polarization to a higher value.

The electrons spins are flipped using an RF-signal at the electron paramagnetic resonance frequency (EPR).

The proton spins are flipped using a RF-signal at the nuclear paramagnetic resonance frequency (NMR).

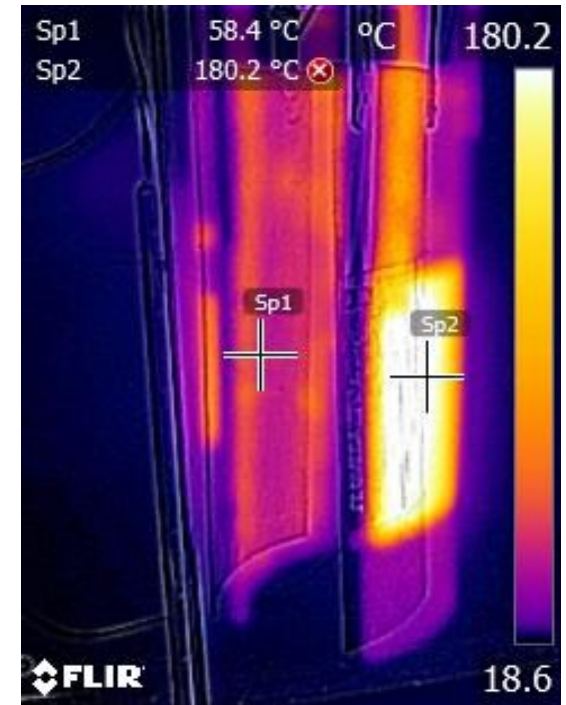
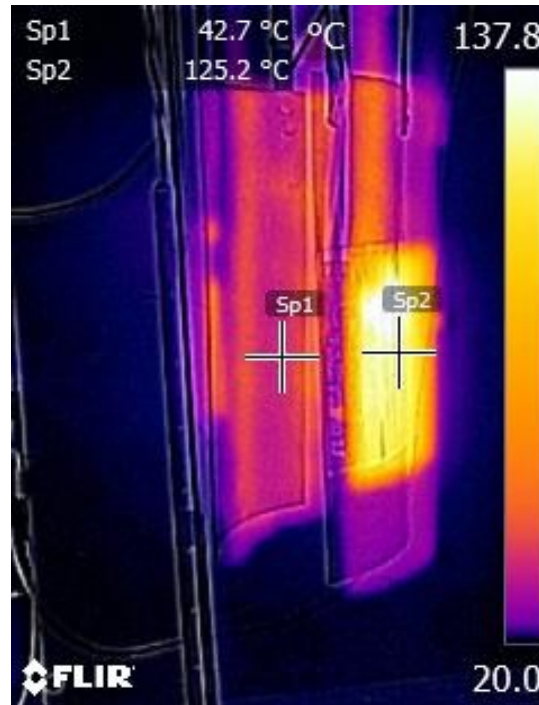
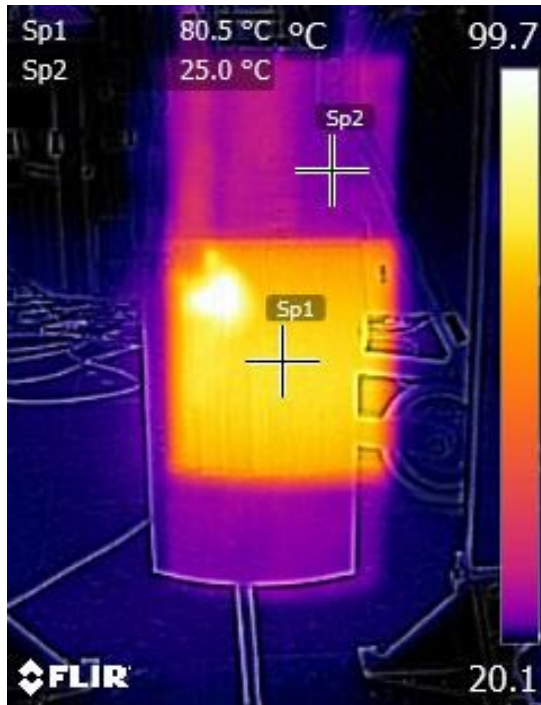
Positive or negative nucleon polarization can be achieved using the proper RF-signal frequency.

Spin flip is B-field independent and requires only a change in RF frequency!



Aligned: $v_e - v_p$
Anti-aligned: $v_e + v_p$

Annealing Plates with Heaters Running



Note that this is the annealing plates running at room temperature in the lab. The heat on the plates will be different in a helium bath.

Target Cooling and Evaporation Refrigerator

The target ladder sits in the nose of the refrigerator cooled by a 1K Helium bath.

Liquid helium at 4K is drawn from a reservoir in the magnet through an insulated jumper and into the separator.

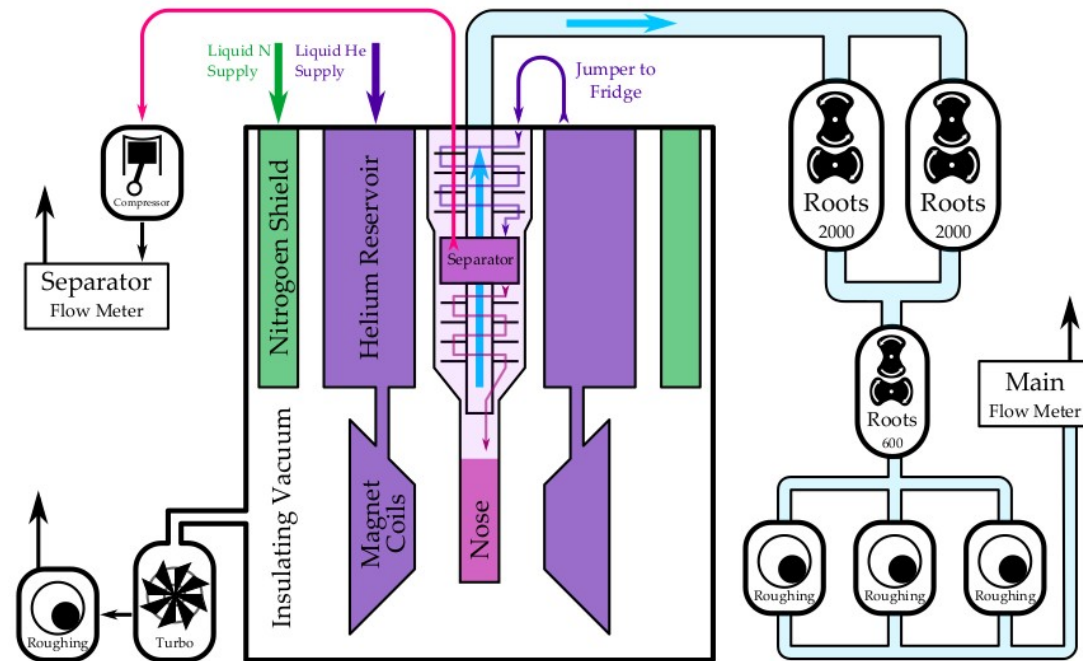
The separator is pumped on by an external pump and through evaporation the Helium temperature is lower to around 3K.

The Helium reaches the nose through either the run valve or the bypass valve.

Evaporated Helium from the nose convectively cools the refrigerator as it is pumped out

The insulating vacuum is $\sim 10^{-7}$ torr and liquid Nitrogen (77K) shield is used to prevent blackbody radiation losses to the outer walls of the cryostat (300K).

High powered pumps are needed to keep low pressure in the nose and deal with the high flow-rate.



Run valve - runs through heat exchanger to further lower the Helium temperature.

Bypass valve - goes directly to the nose.