On polarimetry analysis for GEn-II

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Understanding the calibration constants

Even after getting control of some of the larger issues with calibration constants, there is still quite a bit of scatter among constants that one might naively expect to be equal to one another. Some of the bigger issues include using fast convection, which helps insure that the polarization is fairly uniform throughout the cell. Without fast convection, the afp losses can propagate around the cell, causing considerable variations that have nothing to do with calibration. A lesser but still important issue is being careful to determine calibration constants for specific afp parameters.

Once the larger issues are taken care of, there is still a scatter among calibration constants, typically on the order of 3-3.5%. This is worrisome if the scatter is not well understood, as it prevents us from simply averaging the constants under the assumption that the scatter is random. In fact the 3-3.5% variations are almost certainly associated temperature variations, some of which are intentional (raising and lowering the set point of the oven), and others due to things such as increasing or decreasing the laser power.

In this document I describe a formalism in which temperature and density fluctuations are dealt with by monitoring the ratio of the signals, $\mathbf{R} = S_{pc}/S_{tc}$, due to the pumping chamber and target chamber respectively, where $S_{pc}(S_{tc})$ is the NMR AFP signal from the pumping (target) chamber. I will send with this document an analysis (presented in a spreadsheet) of the eight calibrations of target-cell Hunter during Kin3 that exist at the time of this writing. Without adjustments of the sort described herein, the eight calibrations have a standard deviation of roughly 3.6%. When using the ratios \mathbf{R} to track temperature and density, however, that scatter is reduced by roughly a factor of three. One can then extract a best value associated with a given set of conditions. This best value can subsequently be adjusted for varying conditions, resulting in polarimetry that might approach a level of accuracy better than a 2% level with reasonably well-understood systematic effects.

The analysis presented here for Hunter during Kin3 running (or some other appropriate analysis) needs to be repeated for each cell for which we have data. I don't claim that the formalism presented here is as good as it can be, but it is a good start as we move forward. It really is important that everyone participating in analyzing the polarimetry data dive in and help develop the best approach possible.

The value of the signal ratios

The ratio of the signals in the pumping- and target-chambers provides information that is unambiguously linked to the relative density of gas in the target cells's two chambers at a particular moment in time. Since the pumping chamber and target chamber are in communication with one another, the pressure must be equal in both chambers, and the ideal gas law tells us

$$P = \frac{N_T f_{pc} k_B T_{pc}}{V_{pc}} = \frac{N_T f_{tc} k_B T_{tc}}{V_{tc}}$$

where P is the pressure in the cell, N_T is the total number gas atoms and molecules, k_B is the Boltzmann constant, $f_{pc}(f_{tc})$ is the fraction of the atoms and molecules in the

pumping (target) chamber, $T_{pc}(T_{tc})$ is the temperature in the pumping (target) chamber and $V_{pc}(V_{tc})$ is the volume of the pumping (target) chamber. From this expression we find that

$$\frac{f_{pc}T_{pc}}{V_{pc}} = \frac{f_{tc}T_{tc}}{V_{tc}} \quad \Rightarrow \quad \frac{f_{pc}}{f_{tc}} = \frac{T_{tc}V_{pc}}{T_{pc}V_{tc}} \quad .$$

which turns out to be a particularly useful expression.

The signal $S_{pc}(S_{tc})$ in the pumping (target) chamber can be written

$$S_{pc} = G_{pc} f_{pc} P_{He}$$
 and $S_{tc} = G_{tc} f_{tc} P_{He}$

where all relevant constants have been absorbed into the constants G_{pc} and G_{tc} , and the polarization of the ³He, P_{He} is assumed to be constant throughout the cell (an assumption that is pretty good with fast convection). From this it is clear that the ratio

$$R = \frac{S_{pc}}{S_{tc}} = \frac{G_{pc}f_{pc}}{G_{tc}f_{tc}}$$

It is useful to consider comparing the ratio R and R' corresponding to two different sets of temperatures. In this case, the "ratio of ratios", or super-ratio

$$\mathbf{R} = \frac{R}{R'} = \frac{f_{pc}/f_{tc}}{f'_{pc}/f'_{tc}} = \frac{T_{tc}}{T_{pc}} \frac{T'_{pc}}{T'_{tc}}$$
(1)

where in what follows R will refer to reference point in time and R' will refer to some subsequent point in time.

Absolute and relative temperature determination

Relative temperature determinations — One thing that eqn. (1) gives us is the ability to estimate changes in T_{pc} given knowledge of T_{pc} at some reference point. During production running, it is typically T_{pc} that is changing with time, so it is often the case that $T'_{tc} \approx T_{tc}$. Under this assumption, we have the useful relationship

$$T'_{pc} = \frac{R}{R'} T_{pc} \quad . \tag{2}$$

For example, let us say that we have an estimate of T_{tc} at a particular moment of time, due to any number of different approaches (say, for example, a laser-on/laser-off measurement). We can then use eqn. (2) to estimated the PC's temperature at any subsequent time. The assumption that $T'_{tc} \approx T_{tc}$ is not always perfect, and our estimate of T_{pc} at the reference point may also have its limits. Still, eqn. (2) is useful for particular applications.

Absolute temperature determinations — Another useful case to consider is the situation in which the entire cell is at ambient temperature such that $T_{pc} = T_{tc} = T_{amb.}$. In this case, eqn. (\star) tells us that

$$T'_{pc} = \frac{R}{R'} T'_{tc} = \frac{R_{\text{amb.}}}{R'} T'_{tc}$$
 (3)

where on the right-most side above we have added the subscript "amb." to emphasize that this relationship uses a value of R obtained when the entire cell is at ambient temperatures.

The one limitation of eqn. (2) is that the accuracy of the absolute determination of T'_{pc} necessarily depends on an accurate knowledge of T'_{tc} which is not necessarily such an easy thing to determine. Still, eqn. (3) provides an alternative to the laser-on/laser-off approach for determining T_{pc} .

Relative determinations of f'_{pc} and f'_{tc} in terms of f_{pc} and f_{tc}

p Perhaps the most critical use of the super-ratio **R** is determining the relative changes in time of f_{pc} and f_{tc} . If we have a calibration corresponding to a particular value of, say, f_{tc} , the *correct* calibration constant at a subsequent time will be depend on the ratio f'_{tc}/f_{tc} . Let us define α and β according to

$$f'_{pc} = \alpha f_{pc}$$
 and $f'_{tc} = \beta f_{tc}$.

Since the density of gas in the PC and TC is directly proportional to f_{pc} and f_{tc} , it is also the case that

$$C'_{pc} = \frac{1}{\alpha} C_{pc}$$
 and $C'_{tc} = \frac{1}{\beta} C_{tc}$ (4)

where $C_{pc}(C_{tc})$ is the calibration constant for the PC (TC) at some reference point, and $C'_{pc}(C'_{tc})$ is the calibration constant for the PC (TC) at some subsequent point in time. The relative changes in the calibration constants expressed in eqn. (4) are **absolutely critical** when either comparing calibrations constants, or determining the correct calibration constant for a particular point in time. This last point deserves further emphasis. **Every single NMR measurement requires a different calibration constant adjusted according to eqn. (4).** We can hope that such variations average out, and indeed I believe that they typically do. Counting on such changes averaging out has been our strategy in previous ³He experiments. Whether we do so for GEn-II, however, should be a conscious decision. I suspect that during the periods of time prior to Bill getting his script running, adjustments using eqn. (4) may be quite important.

Determining α and β does not require knowledge of temperature. Given that it is always the case that $f_{pc} + f_{tc} = f'_{pc} + f'_{tc} = 1$, we use eqn. (1) to write

$$\frac{R}{R'} = \frac{f_{pc}/f_{tc}}{f'_{pc}/f'_{tc}} = \frac{(1 - f_{tc})f'_{tc}}{f_{tc}(1 - f'_{tc})}$$

Let $\mathbf{R} = \frac{R}{R'}$ and $f'_{tc} = \beta f_{tc}$. Then

$$\frac{R}{R'} = \mathbf{R} = \frac{(1 - f_{tc})f'_{tc}}{f_{tc}(1 - f'_{tc})} = \frac{(1 - f_{tc})\beta f_{tc}}{f_{tc}(1 - \beta f_{tc})} = \beta \frac{(1 - f_{tc})}{(1 - \beta f_{tc})}$$

and solving for β we find

$$\beta = \frac{\mathbf{R}}{\mathbf{R}f_{tc} + 1 - f_{tc}} \quad . \tag{5}$$

Similarly, if we let $f'_{pc} = \beta f_{pc}$, we have

$$\alpha = 1/(\mathbf{R} - \mathbf{R}f_{pc} + f_{pc}) \tag{6}$$

One advantage in using eqns. (5) and (6) rather than eqn. (2) is that we do not need to assume that $T'_{tc} = T_{tc}$.

When I send this document around, I will include in the pdf a single pdf page showing my most recent results. In the email sending this around, I will also include the spreadsheet itself. The spreadsheet contains the eight 5 G/s 0.2V kin 3 target-cell Hunter calibrations that exist at the time of this writing.

In addition to the raw data from NMR measurements, the spreadsheet requires several inputs, which are entered into the indicated boxes in columns B-F and rows 2-7. The inputs include the volumes and and fill density for the cell in question, in this case, target-cell Hunter. It also includes a value for $d\nu/dB$ in units of kHz/G, which for these calculations is assumed to be that appropriate for 25 G. The value shown is obtained using the Breit-Rabi equation and our usual choice of the $-1 \leftrightarrow -2$ transition. The quantity "cbar" depends solely on fundamental constants and $d\nu/dB$ and is used in computing the %/kHz number.

The inputs entered into cells F3, F4 ad F5 deserve particular attention. These are the temperatures and ratio R corresponding to the specific particular calibration that is being taken as the reference calibration. For the spreadsheet shown, the reference calibration is the fifth, the data for which are given in rows 25 and 26. For the reference calibration, the temperatures are chosen, and the method of choosing them can be whatever we think is best. This also makes it possible to assume different temperatures to see the effect on the resulting calibrations. Note that temperatures entered into cells F3 and F4 also appear (within rounding errors) in cells N25 and O25. Operationally, you do not need to enter any of the temperatures shown in columns N and O by hand. The choice of the reference calibration is established solely by the number entered into cell F5. The thing that establishes the spreadsheet shown as corresponding to the fifth calibration is that the number ended into cell F5 is 0.3153, the ratio shown in cell M25 which is due solely to the raw data from the fifth calibration.

While I don't want to go into too much detail, let me share a few bullet points:

- \bullet In column J I show grad-student Hunter's values for the eight calibration constants. I believe that a single value of %/kHz (0.6401) was used, regardless of changes in temperature or density.
- Again in column J, in rows 37-41, I show the average of the eight calibration constants, their standard deviation, and the fractional scatter of their values, which ends up being 3.6%.
- In columns Z and AA, I show the eight calibration constants adjusted to a common density. The common density chosen in this case is that corresponding to the fifth calibration, that listed in rows 25 and 26.
- In column AA, rows 37-41, I show the average of the eight calibration constants, their standard deviation, and the fractional scatter of their values, which ends up being 1.3%, almost a factor of three reduction compared to when temperature and density adjustments are not made.
- As mentioned earlier, the choice of the PC temperature for the reference calibration has only a mild effect on the resulting best value for the calibration for that cell. This is illustrated in the best values shown in rows 47-50 of column W, corresponding to four assumed temperatures between 250-265C. The total variation of those values is only 0.5% !!! I cannot emphasize enough how fortunate we are that we don't need to know that PC temperature all that well. The values shown in rows 47-50 were generated using the first calibration as the reference, that is, the value 0.2924 (cell M13) was used as the reference ratio R.

- The best calibration values shown in cells M58, M62 and M64 were obtained using the fifth calibration as the reference, the reference used for the spreadsheet as shown, with the reference ratio R=0.31513. Note that the best calibration value corresponding to $T_{pc}=265\mathrm{C}~(2.0419~\%/\mathrm{mV})$ is the value resulting from running the spreadsheet as shown.
- But wait!!! The best calibration values shown when using the first and fifth calibrations as references are way different from one another!!! Should we be worried? NO !!! Any best calibration value is associated with an assumed reference ratio R.
- For example, for the spreadsheet shown, the best value for the calibration, corresponding to the value of R from the fifth calibration, is 2.0419%/mV (cell AA37). The unadjusted calibration for the first calibration is 1.96241%/mV (cell Y14). But for the first calibration, $\beta = 1.03427$ (cell S13). Note that 2.0419%/mV/1.03427 = 1.9742%/mV, only 0.6% different from the value shown Y14.

Conclusions and future plans

One useful thing is that calibration constants do not depend strongly on temperature. One would certainly expect that they would, but by a lucky break, two effects largely cancel one another. If the temperature in the PC is higher, the density will be lower, and we would thus expect the percent polarization per millivolt would be higher. As it turns out, however, kappa0 varies slowly with temperature as well, increasing with increasing temperature. Thus, the %/mV determined for a given set of conditions won't change that much if the assumed temperature of the PC is a little off.

However, if we want to apply a calibration constant to a particular NMR measurement, it is critical that the signal ratio be taken into account; not doing so is likely to result in an error of several percent. Even if you convince yourself that such variations are likely to average out, you could get unlucky and end up quoting a polarization that is off by 3-4% for a set of runs.

To my knowledge, the analysis presented here has not been applied previously. I know that I had not been thinking in these terms until our Kin2 running with Hunter during which I was worried that we did not understand our calibrations at even a fairly gross level. The problem was being aggravated by a number if issues, not the least of which were the huge temperature oscillations that we were experiencing.

Various different strategies have been used during past ³He experiments, and they were probably just fine. Variations such as those discussed above probably end up averaging out over the many runs and calibrations that are performed, particularly when various adjustments were made to account for changing conditions. I believe that the formalism and analysis presented here, however, allows us to greatly reduce our systematic errors, probably even for conditions when the temperature oscillations were large. I have yet to apply this formalism to any set of calibrations other than those shown above, so I am not certain.

Absolute temperature measurements — While I already believe we understand that calibration constant at something like the 1% level, for calibrations are always a good thing. One thing we definitely do NOT understand is the temperature of the pumping chamber under production conditions. Toward that end, once we are don taking beam, it is important that we obtain multiple NMR measurements with the cell at ambient temperatures, that is, under conditions during which the PC and the TC are at the same temperature. Such measurements will allow us to use eqn. (3) to estimate the PC temperature. We should

also do some variation of laser-on/laser-off tests. I know they are not really possible right now in quite the way we have done in the past, but I have some ideas on how we might get equivalent data.

Polarization gradients — In the past, we have worried a great deal about polarization gradients. To first order, we bypass that problem by using the TC pickup coils as our main source of polarimetry. Polarization gradients, however, still come into play as a secondary effect, and I have not addressed that issue at all in what is presented here. If there is a polarization gradient between the PC and the TC, it will effect the ratio R. Since I am proposing using R as a real-time way to adjust the calibration constant for particular measurements, the gradients still come into play at second order. One thing we still need is a better understanding of our convection speeds so that we can account for that effect. While this is an important aspect of our polarimetry analysis, I will not address it further here.

To-do list — Here is a partial list of things I believe we need. I will include superscript † on those items that probably should be addressed sooner rather than later.

- $1.^{\dagger}$ We need to think through how polarization gradients affect the ratio R for individual NMR measurements. They probably aren't a big deal when generating best value calibration constants.
- 2.† We need to think about measurements that might help us get a handle on item 1.
- 3.† We need some variant of laser-on/laser-off measurements.
- $4.^{\dagger}$ We need multiple NMR measurements during which the cell is at ambient temperatures.
- 5. We need to perform an analysis along the lines of what I show above for every set of runs during which we have NMR measurements.
- 6. We need to generate a table of polarization values for every run.
- 7. We need to enumerate and understand any number of other systematic effects not discussed here. For example, how do afp losses affect the polarizations that we assign to each run?
- 8.† What have I forgotten that needs to be done BEFORE wrapping up data taking for Kin3?

Who does what when? — Without sounding too obnoxious, the amount of time I have put into the stuff summarized in this document and the accompanying spreadsheet is huge, and I very much want to hand off the effort. I know I have been a broken record on the need to do more in-depth polarimetry analysis, but I also know that it is hard to know where to start. I am hoping that this document (and spreadsheet) can be a starting point. During the next week we will still have a chance to make additional measurements should we need them. I think people should dive in and get started right away so that we can use our time well.

	A	В	С	D	E	F	G	Н	1	J	К	L	М	N	0	Q	R	S	Т	U	V	W	Х	Υ	Z	AA
1			306.1659		en i	7 00050		,	0.45700																	+
2		V_pc V tt	44.8700		filldensity ref. T pc	7.38659 265.00000		f_pc f tc	0.45720																	
4		V tc	160.9000		ref. T tc	31.50000		1_10	0.04200																	
5					ref. ratio	0.31530			1.00000																	
6		kHz/Gauss	878.7170					cbar	4250.90772																	
7		cbar/(kHz/G)	4.8376					%/mV	0.64229 6.48600									_								-
8								kappa0	6.48600									-								
10																										
11	Time	PC Up	PC Down	TC Down Up	TC Down Down	TC Up Up	TC Up Down	Date	frequencies	Hunter's #'s	PC av. T	C avg.	ratio	T_pc	T_tc	%/kHz	alpha	beta f_	рс	f_tc	calib_pc	calib_tc	avg. calib_pc	avg. calib_tc	adj. calib_pc	adj. calib_tc
12	2212011046	5.525137	5.442283	18.980548	18.521545	17.379254	40 000700	D 4 2022	55.22		5.4837	18.7510	0.2924	285.707	31.50	0.65144	0.95931	1.03427	0.43860	0.56140	6.55984	1.91841				
	2212011048	4.86416		17.14886			14.993543	Dec. 1, 2022	52.22		4.8420	16.9546		205.707	31.50		0.95931	1.03427	0.43000	0.36140	7.02557		6.79270	1.96241	6.51632	2.02967
15																										
16	2212021315	5.816757 5.156175	5.701842 5.046362	20.135772	19.660374	18.473995 16.474259	17.797058	Dec. 2, 2022	58.67 55.16	1.931	5.7593 5.1013	19.8981 17.8792	0.2894	288.676	31.50 31.50	0.65271	0.95375	1.03896	0.43606	0.56394	6.64913 7.05772	1.92452 2.01369	6.85342	1.96911	6.53643	2.04582
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19	2212021336	4.952243	4.894996	16.214205	15.750406	14.694073		Dec. 2, 2022	49.5 46.98		4.9236	15.9823	0.3081	271.222	31.50		0.98742	1.01060	0.45145	0.54855	6.48545	1.99795	6.70709	0.00070		2.06034
21	2212021338	4.382307	4.365696	14.74799	14.399537	13.117729	12.528096	1	46.98	2.023	4.3740	14.5738	0.3001		31.50						6.92873	2.07951	6.70709	2.03873	6.62269	2.06034
22	2212021509	4.233968	4.183006	13.627886	13.271718			Dec. 2, 2022	41.58		4.2085	13.4498		267.030	31.50		0.99586	1.00349	0.45531	0.54469						
23	2212021511	3.734199	3.675326	12.390806	12.129983	11.105159	10.742575	5	39.91	2.031	3.7048	12.2604	0.3022		31.50						6.92902	2.09376	6.64196	2.04112	6.61446	2.04824
25	2212021526	3.631483	3.574341	11.584929	11.271837		10.22971	Dec. 2, 2022	36.37		3.6029	11.4284		265.034	31.50		0.99993	1.00006	0.45717	0.54283						
26	2212021528	3.214979	3.143303	10.59456	10.243765	9.452294	9.13463	1	34.15	2.068	3.1791	10.4192	0.3051		31.50	1					6.89955	2.10522	6.69167	2.07465	6.69121	2.07477
28	2212071254	6.373631	6.292193	22.302387	21.862429	20.83063	20.215213	Dec. 7, 2022	62.77		6.3329	22.0824	0.2868	291.349	31.50	0.65384	0.94879	1.04313	0.43379	0.56621	6.48070	1.85857				
29	2212071256	5.639884		20.143003	19.710434		17.697889		59.3		5.5829	19.9267			31.50						6.94495	1.94577	6.71283	1.90217	6.36909	1.98421
30	2212071327	5.355194	5.276191	17.222098	16.848749	15.63613	16 160422	Dec. 7, 2022	52.93		5.3157	17.0354	0.3120	267.771	31.50	0.64354	0.99436	1.00475	0.45462	0.54538	6.40793	1.99952				-
32	2212071329	4.701206	4.632671	15.483522	15.197424		13.545247	Dec. 7, 2022	49.48		4.6669	15.3405		201.111	31.50		0.88430	1.00473	0.43402	0.34330	6.82297		6.61545	2.03761	6.57812	2.04730
33																										
34	2212071401 2212071402	4.52422 3.995585	4.458729 3.956579	14.530348 13.168845	14.24977 12.954378	13.221986 11.919391	12.761723	Dec. 7, 2022	44.51 42.21		4.4915 3.9761	14.3901	0.3121	267.697	31.50 31.50		0.99451	1.00463	0.45469	0.54531	6.37709 6.83146		6.60427	2.03500	6.56799	2.04442
36	ZZ IZOT IHOZ	0.000000	0.000075	10.100040	12.004070	11.010001	11.401000		72.21	2.024	0.0101	10.0010	0.0044		01.00						0.00140	2.07000	0.00421	2.00000	0.00700	2.04442
37									average	1.98675														average	6.56204	2.04185
38																										
40									std. deviation	0.07071								-						std. dev.	0.09515	0.02670
41									% scatter	0.03559														% scatter	0.01450	0.01307
42																										
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49								1													260C =>	1.94816				
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