Description of NMR Plots

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nmr_deut_te_4plot

This slide contains 4 plots of the evolution of the target thermal equilibrium NMR signal. The top left plot is of the baseline which is taken off resonance. We move the target field down enough to remove the signal from the width of the Q-curve (1% for protons, 3% for deuterons in ND_3). The top right plot is the raw TE signal before baseline subtraction. This is what is read back to our target DAQ. Notice you cannot see the signal with the naked eye (see overlay of baseline and raw te signal on **nmr_deut_te_rawtedif.eps**). The bottom left plot is of the baseline subtracted signal. It is essentially the top left plot subtracted from the top right plot. You can barely make out the bumps of the deuteron peaks. The signal is askew because the baseline signal and the raw signal never quite have the same curvature, leaving a residual curve. This is because the presence of the signal warps the curvature of the raw signal, but also the baseline is taken at a different field, so there is some effect from this as well. The bottom right plot is the "poly-subtracted" signal. A third-order polynomial is fit to the wings of the bottom left plot and then subtracted from the baseline-subtracted signal. This step can be difficult since the limits of the wings are hard to determine for small signals. Also, positioning of the peak can shift some when the field has been moved around, and this will also affect where the edges of the signal are. Finding appropriate fit regions is a painstaking offline process.

The baseline subtracted plot and poly-subtracted plot can be viewed on individual slides (**nmr_deut_te_bsubt.eps** and **nmr_deut_te_poly.eps**, respectively).

nmr_deut_enh_4plot

This slide is the same as for the te, but with enhanced signals. Here you can clearly see the deuteron peaks in the raw signal, and the residual curve is small for the baseline subtracted signal. Units on the y-axis are millivolts, so you can see how much larger this signal is compared to the te. The poly-subtracted signal looks extremely flat, and is compared to the rest of the signal. Refitting of the wings in offline analysis is not nearly as important for enhanced signals.

Individual plots of these signals can be found on the slides:

- **nmr_deut_enh_baseline.eps**
- **nmr_deut_enh_raw.eps**
- **nmr_deut_enh_bsubt.eps**
- **nmr_deut_enh_poly.eps**

nmr_deut_enh_poly_close

This plot shows a close-up of the poly-subtracted enhanced deuteron signal. It reveals some of the inadequecies of the fitting procedure. On the low frequency side, there is clearly something not right. This comes from the difficulty in fitting the wings. For enhanced signals, a straight percentage of each wing is taken for fitting (making sure not to come close to cutting off the signal and not picking up any of the edge noise). But this is not perfect and often there is a small wiggle left near where the deuteron pedestal meets the flat part of the Q-curve. However, the scale of this wiggle is tiny and it's effect on the total signal area is too small to measure (or worry about).

deuteron nmr basics

Just thought I'd include some basics on the deuteron nmr signals. The shape of the deuteron in ND_3 is peculiar. It is spin 1, but due to the lattice structure of the molecule, the quadrupole interaction with the electric field gradient causes this splitting of the transitions. The right (higher frequency) peak and left (lower frequency) pedestal correspond to the m=+1 to m=0 transition. The left peak and right pedestal corresponds to the m=0 to m=-1 transition. Before technology existed to sufficiently measure the thermal equilibrium signals (we've seen how small they can be), the enhanced polarization was determined from peak height ratios. The ratio of the intensities of each transition can be used to determine polarization. If a Boltzmann distribution of spins across magnetic sublevels can be assumed, the polarization is given by

$$P = \frac{R^2 - 1}{R^2 + R + 1} \tag{1}$$

where R is the ratio of transition intensities (R>1.0). This method is still used sometimes as a redundancy check on our calibrated measurement (or when we aren't allowed to take a te and have to polarize blindly). Other deuterated materials with a different lattice structure do not necessarily have this same sort of signal shape. ^{6}LiD, for instance, has a face-centered-cubic (fcc) structure and therefore has no interaction between the quadrupole moment and the electric field gradient. Both transitions have the same frequency and lie on top of each other producing a very sharp, single peak resonance.

data acquisition basics

Each of the signals you see on these plots, either te or enhanced, is a single data point composed from several sweeps across the resonance frequency. Each measurement we make (which corresponds to one polarization data point in the data stream) comes from an averaged response from 200-1000 sweeps, depending on the signal type. Typically a deuteron TE signal would be made from 1000 sweeps. Deuteron enhanced data can be anywhere between 200 and 500 sweeps (I think most Gen data was taken at 500 sweeps). A set of 500 sweeps generally took about 40 seconds to measure.

For the TE measurement, several of these individual measurements were taken over a period of time when both the area and temperature in the target cavity seemed stable. The calibration constant is calculated from an average area and temperature over this period of time with the associated statistical error from fluctuations in individual measurements.