

## Tensor Polarization Enhancement in Nuclear Solid Targets

S. Bültmann, D. G. Crabb, Y. Prok (*University of Virginia*)

April 18, 2000

The deuterium nucleus has spin  $I = 1$ . In the presence of a magnetic field, an ensemble of spins is splitting into  $(2I + 1 = 3)$  energy sublevels  $m$ . For a spin-1 ensemble, the relative occupation of the sublevels is determined by two quantities, usually the vector polarization

$$P = \frac{N_{+1} - N_{-1}}{N_{+1} + N_0 + N_{-1}} \quad (-1 \leq P \leq +1)$$

and the alignment or tensor polarization

$$A = \frac{N_{-1} - 2N_0 + N_{+1}}{N_{+1} + N_0 + N_{-1}} \quad (-2 \leq A \leq +1),$$

where  $N_m$  is the population of the respective sublevels.

The vector polarization can be measured by Nuclear Magnetic Resonance (NMR), where the integral of the resonance line is proportional to the strength of the transition between the sublevels and hence proportional to the vector polarization. The tensor polarization can be obtained only from the relative strength of the two transitions between  $(m = +1 \leftrightarrow m = 0)$  and  $(m = 0 \leftrightarrow m = -1)$ . This requires the measurement of the two individual transitions.

In most solid materials for polarized targets these individual resonance lines perfectly overlap and do not allow the separation of the individual transition strengths. However, in the case of deuterated solid ammonia and alcohols, the deuteron electric quadrupole moment is interacting with the electric field gradient of the molecule, thereby leading to frequency shifted resonance lines of the two transitions. For ammonia or alcohols, the resonance lines are overlapping, but asymmetric with their maxima at different frequencies. In Fig. 1 the theoretical line shape from a model [1] of the deuteron resonance signal is given.

Measured line shapes of different target materials will deviate slightly from the model due to different molecular environments. A fit of the model to the measured line shape allows to extract the two transitions resonance lines separately. This determines the relative population of the magnetic sublevels together with the vector polarization.

Tensor and vector polarization of an undisturbed spin system in a magnetic field follow the Boltzmann statistics. The natural vector polarization is then calculable from the Brillouin function and is given by

$$P_0 = \frac{4 \tanh(\frac{\mu_d B}{2kT})}{3 + \tanh^2(\frac{\mu_d B}{2kT})} \quad (-1 \leq P_0 \leq +1).$$

In this case the tensor polarization is related to the vector polarization by

$$A_0 = \frac{4 \tanh^2(\frac{\mu_d B}{2kT})}{3 + \tanh^2(\frac{\mu_d B}{2kT})} = 2 - \sqrt{4 - 3P_0^2} \quad (0 \leq A_0 \leq +1).$$

Starting from a high vector polarization, where either the  $m=+1$  or the  $m=-1$  sublevels are artificially overpopulated, a tensor polarization beyond the natural one can be obtained by inverting the populations of the highly populated sublevel and the  $m=0$  sublevel. This results in scarcely populated  $m=\pm 1$  sublevels, and hence low vector polarization, and an almost entirely filled  $m=0$  sublevel. The resulting tensor polarization would be close to  $A = -2$ . This can be achieved, at least partially, by adiabatically sweeping high power RF over half of the resonance line, either from the low or high end side towards the centre (Larmor) frequency. For positive vector polarization it is more efficient to sweep over the higher frequency half, leading to an inversion of the  $m=+1$  and  $m=0$  sublevels, while for negative vector polarization it is the lower half (inversion of  $m=0$  and  $m=-1$  sublevels). The inversion of the sublevels will not be complete, because the two resonance lines do overlap and hence a fraction of the spins from the  $m=0$  sublevel undergo a induced transition into the  $m=-1$  sublevel. Secondly, a fraction of the spins from the  $m=+1$  sublevel, being close to the maxima of the other transition, are outside the frequency sweep. An extension of the sweep width would also induce the unwanted transition of spins from the  $m=0$  into the  $m=-1$  sublevel.

This process is very similar to the adiabatic fast passage (AFP) method to reverse vector polarization, which has been studied and described in detail in [2]. There, instead of a half sweep, the RF is swept additionally once through the entire resonance line. The efficiency of the reversion of the  $m=\pm 1$  sublevels was shown to be about 90% [2]. The additional equipment needed are an additional RF coil surrounding the target, a controllable RF sweep generator, and if necessary an amplifier.

A considerably less effective method to achieve limited enhanced tensor polarization is to equalize two sublevels by RF saturation. Starting from the high vector polarization described above, the resonance signal of a negatively polarized ensemble has a large transition peak at low frequency ( $m=0 \leftrightarrow m=-1$ ) and a small transition peak at high frequency ( $m=+1 \leftrightarrow m=0$ ). An example of a polarized deuteron signal in ammonia with  $P = -0.41$  is shown in Fig. 2 by the solid line. The corresponding tensor polarization is  $A = +0.13$ , assuming Boltzmann distribution among the three sublevels. This assumption also leads to the relative occupancy of the sublevels,

$$\frac{N_{+1}}{N_0} = \frac{N_0}{N_{-1}} = e^{\frac{\mu_d B}{kT}} = 0.517617.$$

In an exploratory experiment the RF output of a RF generator was directly connected to the NMR coil inside the target. The unattenuated high RF power was swept 400 times through the centre of the of the ( $m=0 \leftrightarrow m=-1$ ) transition in a range of  $\pm 30$  kHz (40 channels), leading towards an equalization of the two sublevels. The resulting resonance signal is shown in Fig. 2 by the dashed line. Its vector polarization is now  $P = -0.34$ . The ( $m=0 \leftrightarrow m=-1$ ) transition almost completely disappeared ( $N_0 \simeq N_{-1}$ ), while the ( $m=+1 \leftrightarrow m=0$ ) transition is now enhanced due to the higher populated  $m=0$  sublevel. This method cannot be fully efficient because of the overlapping transitions, visible in the pedestals under the respectively opposite transition. Assuming now a complete equalization of the  $m=-1$  and the  $m=0$  sublevels one obtains a theoretical value for the

tensor polarization of  $A = -0.27 \stackrel{!}{=} -|P|$ , together with the above given relative occupancies. One can see, that the sign of the alignment is reversed, however, the measured vector polarization does not fully agree with the theoretical expectation, because of the limited usage of the method.

- [1] The Spin Muon Collaboration (SMC), C. Dulya et al.,  
*A line shape analysis for spin 1 NMR signals*,  
Nucl. Instr. and Meth. A 398 (1997) 109 – 125.
- [2] P. Hautle et al.,  
*Polarization reversal by adiabatic fast passage in various polarized target materials*,  
Nucl. Instr. and Meth. A 356 (1995) 108 – 110.

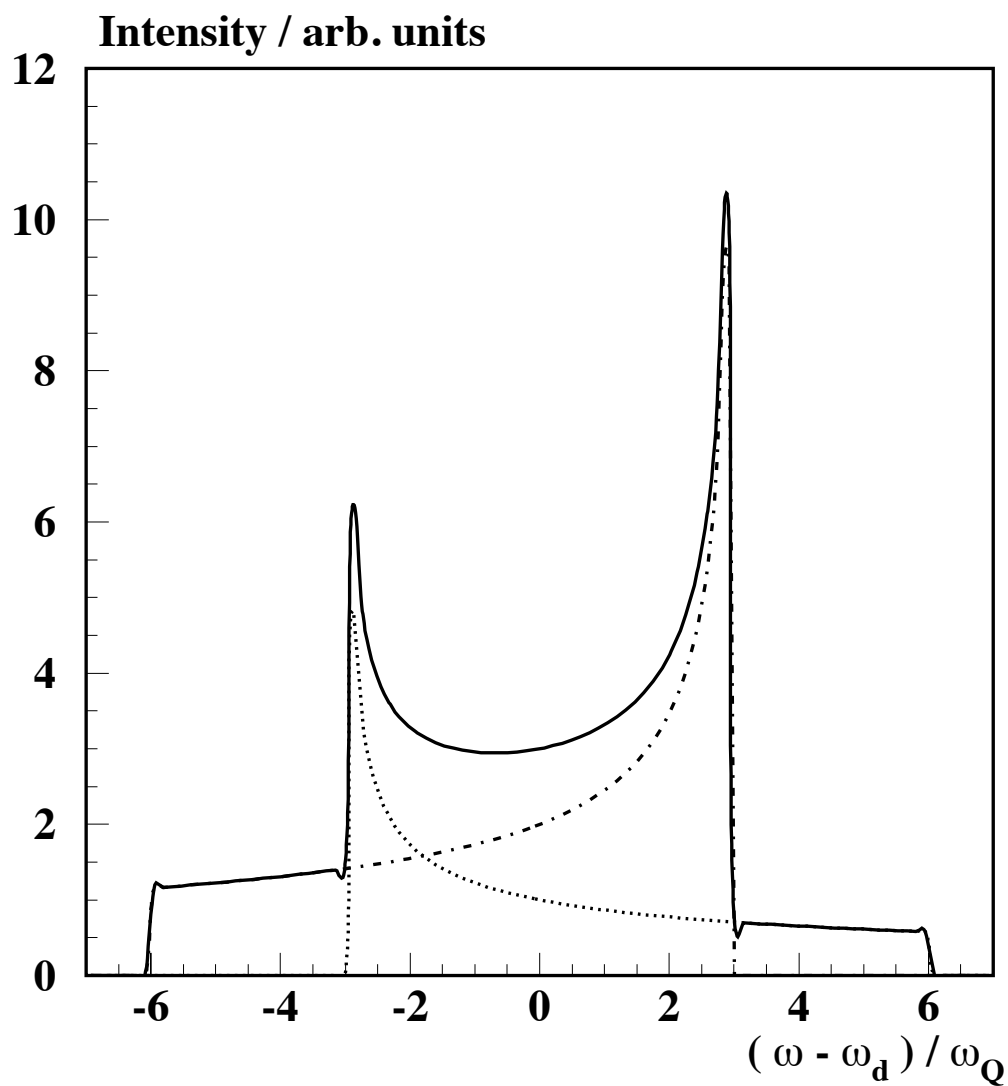


Figure 1: A model calculation of the two transitions in the deuteron spin system. The resulting resonance line shape is given by the full line.  $\omega$  is the frequency,  $\omega_d$  is the deuteron Larmor frequency, and  $\omega_Q$  is the quadrupole interaction frequency. (From [1])

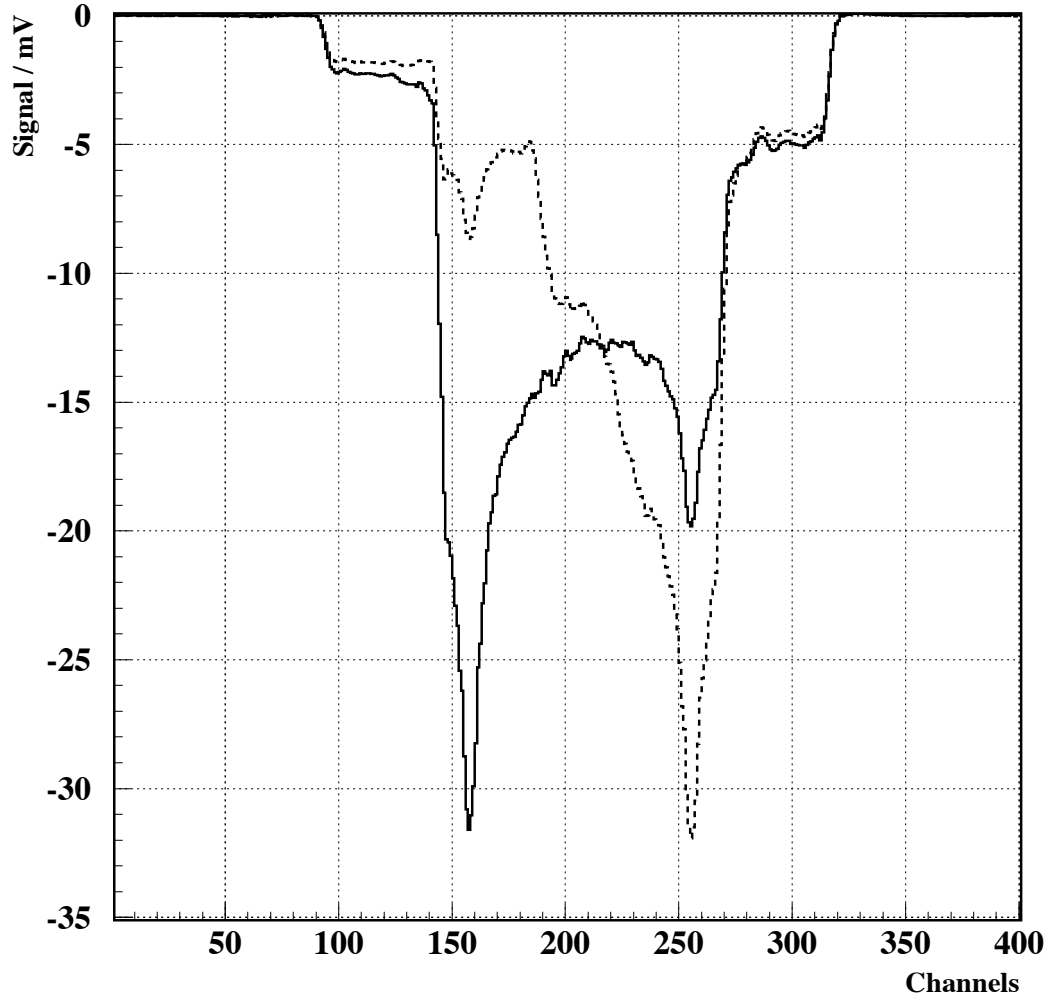


Figure 2: Deuteron resonance signal in solid ammonia of  $P = -0.41$  (solid line) before RF saturation of the low frequency transition and after with  $P = -0.34$  (dashed line). The 400 channels correspond to a total sweep width of  $\pm 300$  kHz around the centre frequency of 32.709 MHz.