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TENSOR POLARIZATION STUDIES IN A SINGLE CRYSTAL OF ND3

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ABSTRACT

A method to enhance the tensor polarization[1] of a polarized deuteron target by reducing the vector polarization by means of a RF transition saturation technique is shown. For this, a single crystal of deuterated ammonia was polarized to a degree of P=20 %. The tensor polarization could be increased from A=0.03 to A=0.14.

1. Introduction to the Method

Since the deuteron is a spin 1 particle, the deuteron energy level in a magnetic field splits into three sublevels $m = -1, 0, +1$ (Zeeman Effect,$\Delta E_1 = \Delta E_2$), according to the spin orientation (Fig. 1). The population of the energy levels is due to the Boltzmann law, a good 'thermal' contact between the deuteron spins provided. At this stage, the quadrupole splitting is neglected. Transitions e.g. from $m = +1$ to $m = 0$ as well as from $m = 0$ to the $m = -1$ level are used to detect polarization by an alternating transversal magnetic field via Nuclear Magnetic Resonance (NMR). For a Boltzmann distribution the ratio R of both transitions (associated with the peak ratio of a given polarization signal) may be used to determine the vector polarization P by equation (1) [1].

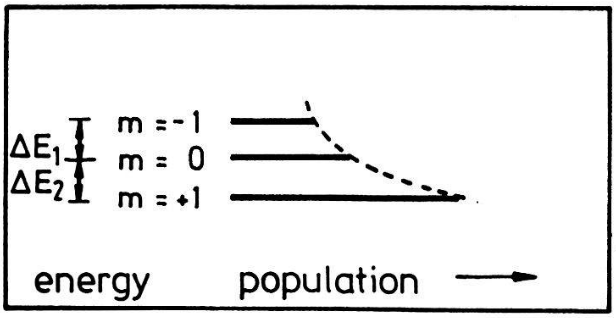


Fig.1: The sublevel population of the deuteron spin system

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

Independent from these considerations P is given by (2):

$$P = \frac{(n_- - n_0) + (n_0 - n_+)}{n_- + n_0 + n_+} \tag{2}$$

and the tensor polarization A as

$$A = \frac{(n_- - n_0) - (n_0 - n_+)}{n_- + n_0 + n_+}$$

$$= 2\frac{\frac{(n_- + n_+)}{2} - n_0}{n_- + n_0 + n_+} \tag{3}$$

where (3) indicates that A is two times the population average between the upper and the lower level minus the population of the intermediate level.

[1] alignment, $A = \sqrt{2}t_{20}$, Madison convention

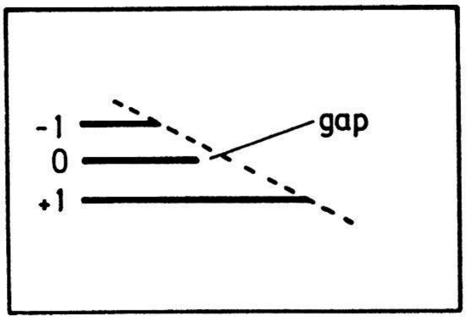


Fig.2 : The gap width is proportional to the tensor pol. A

Enhancing the gap between the dotted line and the population of the intermediate level, as indicated in fig.2 would mean an enhancement of the tensor polarization. The idea of RF saturation is to equalize e.g. the upper and the intermediate level population (fig. 3).
Thus one achieves a remarkably higher positive tensor polarization.
A similar result is reached by doing the same to the lower levels, thus obtaining a negative tensor polarization (fig. 4).

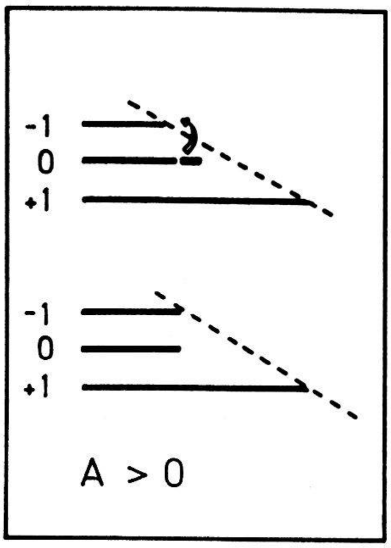


Fig.3 : Enhancing the tensor polarisation by saturation of the upper transition

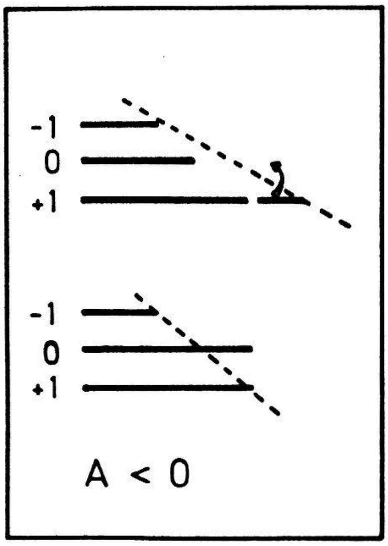


Fig. 4: Enhancing A by saturation of the lower transition.

In the first case the tensor polarization A_{final} is equal to

$$A_f = \frac{R+\frac{1}{2}}{R+1} \cdot P_i \tag{4}$$

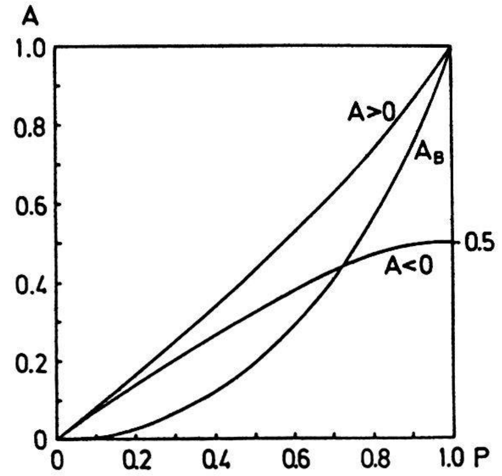
where P_i is the initial vector polarization and R the transition ratio. From the eqs. (2),(3) it is obvious that for either : $n_{-1} = n_0$ or for the case $n_0 = n_{+1}$ one obtains:

$$|A_f| = P_f \tag{5}$$

the final vector polarization P_f being less than the initial one. The tensor polarization A_{final}, however, is much higher than the one (eq.6) due to the Boltzmann distribution:

$$A = 2 - \sqrt{4 - 3P^2} \tag{6}$$

This equation is valid for a thermal equilibrium of the deuteron spin system and is commonly used for determining A from P. Fig. 5 gives a survey of the accessable degrees of A_f, starting with a certain



degree of P.
Though all figures refer to a positive vector polarization, the results are as well valid for a negative one.
However, fig.5 corresponds to a situation, in which only *one* of the two transitions is saturated. For this $\Delta\ E_1 \neq \Delta\ E_2$ (see fig.1) is required. Now the el. quadrupole interaction has to be taken into account.

Fig. 5: Tensor polarization limits *without* (A_B) and *with* transition saturation ($A < 0,\ A > 0$).

2. Deuteron Polarization Signal

The deuteron signal shape can be understood as a superposition of gaussian signals due to the relative orientation (angle θ) between a molecular electric field gradient at the location of each deuteron and the deuteron's electric quadrupole moment. The quadrupole splitting for a spin 1 particle is described by eq.(5):

$$\delta E_Q = \delta(3\cos^2\theta - 1)(3m^2 - 2) \tag{5}$$

$\delta = \frac{1}{8} e \cdot Q \cdot \psi_{ZZ}$
e elementary charge
Q quadrupole moment of the deuteron=$2.73 \cdot 10^{-27} \cdot e\ cm^2$
$\psi_{zz} = \frac{dE_z}{dz}$; E el.field strength

In a polycrystalline or a amorphous sample all possible angles occur whereas in a single crystal the orientation between deuterons and el. field gradients are restricted to a few angles of θ.

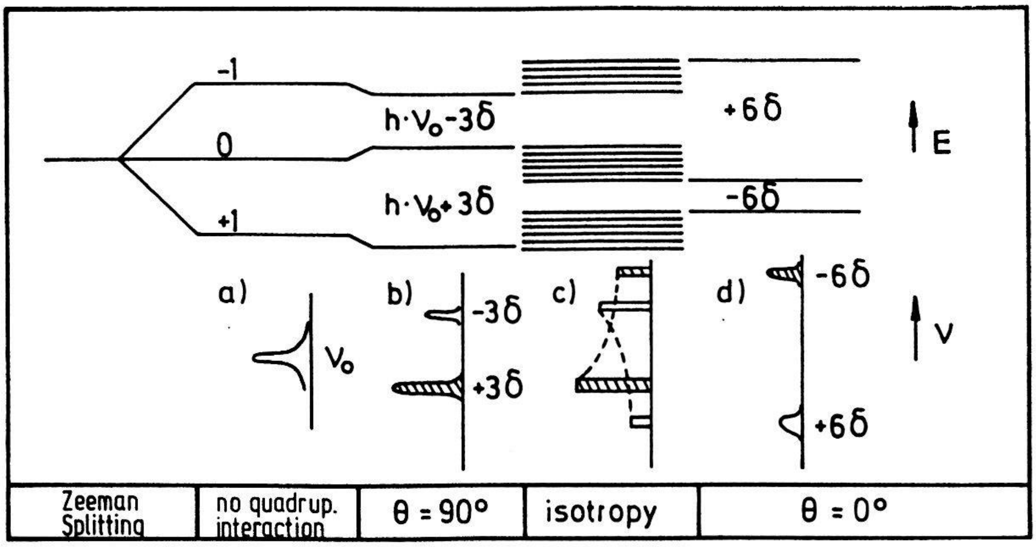


Fig.6: The components of a deuteron signal.
(a) Zeeman splitting $\Delta E_1 = \Delta E_2$,
(b) for a certain angle $\theta = 90^0$ $\Delta E_1 \neq \Delta E_2$,

(c) for a amorphous sample

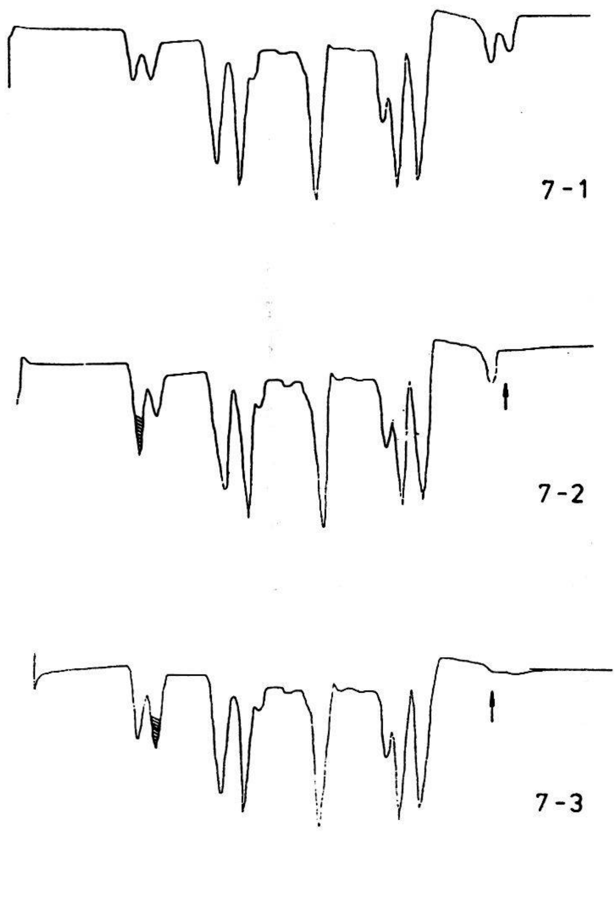
-6δ to -3δ	$\Delta E_1 \neq \Delta E_2$
-3δ to $+3\delta$	$\Delta E_1 = \Delta E_2$
$+3\delta$ to $+6\delta$	$\Delta E_1 \neq \Delta E_2$,

(d) for a certain angle $\theta = 0^0$ $\quad \Delta E_1 \neq \Delta E_2$.

The energy range which is covered is 12δ, a transition mixing occurs between -3δ and $+3\delta$. For a detailed discussion of the signal shape see e.g.[2]. The peak height of the detected deuteron signal is proportional to the population difference of the energy levels, the smaller peak belongs to the $m = 0 \leftrightarrow m = -1$ transition (in case of a positive vector polarization, Boltzmann distribution provided). Results on transition saturation in polycrystalline sample have already been reported. By starting with 36% vector polarization, the tensor polarization went up from 0.10 to 0.16 [3].

3. Single Crystal and Polarization Results

Unfortunately, the success of the saturation technique is limited by the mixing of transitions in the -3δ to $+3\delta$ region of the deuteron signal (fig.6). Saturating the upper $m = 0 \leftrightarrow m = -1$ transition implies a simultaneous saturation the lower $m = +1 \leftrightarrow m = 0$ transition, which diminuishes the gain of this technique. For this reason, monocrystalline ND_3 was prepared [5]. ND_3 crystals consist of cubic unit cells, showing a high symmetry according to one space diagonal. If the crystal is orientated with this diagonal parallel to the magnetic field, a simple polarization signal is expected. It will consist of 8 well resolved peaks due to a high symmetry in θ, and no transition mixing will occur. An arbitrarily orientated crystal will produce 24 peaks, about equally high. This is due to 12 possible orientations of field gradients ($N \leftrightarrow D$ directions) since a unit cell consists of four ND_3 molecules. In case of fig.7 the number of angles were restricted to 11 peaks due to some lower symmetry. This was obtained by rotating the crystal perpendicular to the magnetic field from an arbitrary position to a position with good peak resolution.



The diameter of the ND_3 crystal was 8 mm. The crystal was embedded in a glass tube of 25 mm length. The radicals, necessary for the dynamic nuclear polarization process were produced by irradiation [4]. The polarization measurement was performed at a temperature of about 0.2 K and a magnetic field of 2.5 T. The RF was fed in via the cylindric NMR coil bearing the sample. To the central peak both transitions contribute. For this reason no RF was applied to that frequency region.

In fig. 7-1 a mean vector polarization of 20% was calculated from eq.(1), the different ratios of R were taken into account. From the measurement of the T.E. (thermal equilibrium) signal at 1 K a polarization P of 15 % was indicated. The results are in agreement within errors, since there was no baseline correction of the signals. The derivation to the expected polarization value of 30% (polycrystalline sample [4]) is probably due to a bad cooling of the ND_3 block in the glass tube.

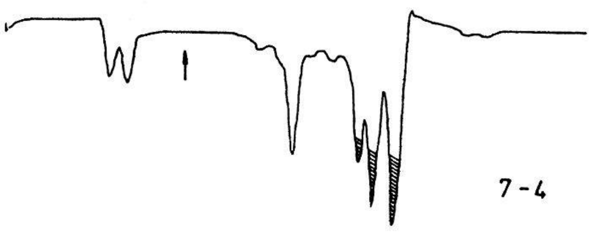


Fig. 7-2 and fig. 7-3 show NMR signals after two RF irradiation periods of typically 10 sec lengths at frequencies of 16.490 and 16.460 MHz. The signal shown in fig 7-4 occured after a ten second frequency sweep from 16.340 to 16.260 MHz. The output voltage of the load matched oszillator was 1 V (peak to peak).

A tensor polarization of 0.14 was calculated. For this the assumption was made that only the intermediate peak consists of contributions of *both* transition types. A computer study to decide this will be completed soon [5][6].

In future there will be efforts to get a higher vector polarization by a better cooling of the crystal. In addition, we have to learn to determine the symmetry axis of the crystal. A complete transition separation at a given vector polarization of 30% will lead to a tensor polarization of 0.24, which would allow us an efficient measurement of the asymmetry T_{20} of the deuteron photodisintegration reaction.

4. References

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Rapporteur's report, Session (K), W. Wenckebach:

The aim of the work is to create a high tensor polarization of the deuterons while the vector polarization is zero. The group at Bonn tries to achieve this result by DNP and subsequent saturation of one of the two $\Delta I_z = \pm 1$ transitions of the deuterons. As this is difficult in a glassy material single crystals of ND_3 were grown. It was tried to perform an adiabatic passage on the NMR line instead of saturating it, but the results were not better than with saturation.

It appears that high tensor polarizations can be maintained for long periods of time, so cross-relaxation between NMR-lines is not very important for its decay.

It would be worthwhile to calculate the maximum tensor polarization that can be achieved by adiabatic means, starting at a given vector polarization obtained by DNP. This would allow a comparison of the results obtained thus far and the theoretical limit.