

## Evolution of Spin Density Matrix in Pure NQR

M. S. Krishnan and B. C. Sanctuary

Department of Chemistry, McGill University,  
Montreal, P.Q. Canada

Z. Naturforsch. **42a**, 907–908 (1987);  
received May 9, 1987

The exact time evolution of the spin density matrix for pure NQR of a spin  $I = 3/2$  system under an asymmetric quadrupole Hamiltonian is given. This extends the results of a previous publication\*.

In our earlier paper [1] entitled “A Spherical Tensor Method for Pure NQR”, Tables 2A and 2B contain a number of errors which, if used to calculate the evolution of the density matrix for a spin  $3/2$  under the influence of an electric quadrupole interaction with a non-negligible asymmetry term  $\eta$ , will lead to incorrect results.

In this note, as in [1] the Hamiltonian

$$H_{\text{asymm}} = \frac{e^2 Q q}{4I(2I-1)} \left[ (3I_z^2 - I^2) + \frac{\eta}{2} (I_+^2 + I_-^2) \right] \quad (1)$$

and the density operator expanded in a spherical tensor operator  $\mathcal{Y}^{(k)}(I)$  basis

$$\sigma(t) = \frac{1}{2I+1} \sum_{k=0}^{2I} \sum_{q=-k}^k \mathcal{Y}^{(k)}(I) \Phi_q^{(k)}(t) \quad (2)$$

are used. The polarizations  $\Phi_q^{(k)}(t)$  are calculated from any initial conditions as

$$\Phi_q^{(k)}(t) = \sum_{k'q'} M_{qq'}^{kk'}(t) \Phi_{q'}^{(k')}(0). \quad (3)$$

The matrix elements  $M_{qq'}^{kk'}(t)$  obviate the need for Tables 2A and 2B in [1], since (3) gives a new and useful result for the full evolution in [1] of a spin  $3/2$  in NQR.

The  $M$ 's are found by a similar procedure as outlined in [1]. Using the symmetry

$$M_{qq'}^{kk'} = (-1)^{k+k'} M_{-q-q'}^{kk'} = (-1)^{k+k'} M_{q'q}^{k'k}$$

Reprint requests to Prof. B. C. Sanctuary, Department of Chemistry, McGill University, 801 Sherbrooke St. West, Montreal P.Q./Canada.

\* Z. Naturforsch. **41a**, 353 (1986).

Table 1.

$$\begin{aligned} M_{||}^{||} &= \frac{2(2\eta^2+3)}{5B^2} + \frac{(\eta^2+9)}{5B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \\ M_{||}^{+2} &= \frac{3}{\sqrt{5}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \\ M_{||}^{+3} &= \frac{\sqrt{3}}{5\sqrt{2}B^2} \left[ (2-\eta^2) + (\eta^2-6) \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right]; \\ M_{+-}^{+-} &= \frac{6\eta}{5B^2} \left( 1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right); \\ M_{+-}^{-2} &= \frac{\eta}{\sqrt{5}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \\ M_{+-}^{-3} &= \frac{\sqrt{6}\eta}{10B^2} \left( 1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right); \\ M_{+3}^{+3} &= \frac{-3\eta}{\sqrt{10}B^2} \left( 1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right); \\ M_{+3}^{-3} &= \frac{\eta^2}{\sqrt{10}B^2} \left( 1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right); \\ M_{++}^{++} &= \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \quad M_{++}^{+3} = \frac{\sqrt{6}}{\sqrt{5}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \\ M_{++}^{-2} &= 0; \quad M_{++}^{-3} = \frac{\sqrt{3}\eta}{\sqrt{10}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \\ M_{+3}^{+3} &= -\frac{\eta}{\sqrt{2}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \quad M_{+3}^{-3} = 0; \\ M_{+3}^{+3} &= \frac{(7\eta^2+18)}{10B^2} + \frac{3(\eta^2+4)}{10B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \\ M_{+3}^{-3} &= \frac{-6\eta}{5B^2} \left( 1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right); \\ M_{+3}^{+3} &= \frac{\sqrt{3}\eta}{\sqrt{5}B^2} \left( 1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right); \\ M_{+3}^{-3} &= \frac{\sqrt{3}\eta^2}{2\sqrt{5}B^2} \left( 1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right); \\ M_{33}^{33} &= \frac{(\eta^2+6)}{2B^2} + \frac{\eta^2}{2B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \quad M_{33}^{-3} = 0; \\ M_{00}^{23} &= 0; \quad M_{00}^{11} = \frac{\eta^2+15}{5B^2} + \frac{4\eta^2}{5B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \end{aligned}$$



Dieses Werk wurde im Jahr 2013 vom Verlag Zeitschrift für Naturforschung in Zusammenarbeit mit der Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V. digitalisiert und unter folgender Lizenz veröffentlicht:  
Creative Commons Namensnennung-Keine Bearbeitung 3.0 Deutschland Lizenz.

Zum 01.01.2015 ist eine Anpassung der Lizenzbedingungen (Entfall der Creative Commons Lizenzbedingung „Keine Bearbeitung“) beabsichtigt, um eine Nachnutzung auch im Rahmen zukünftiger wissenschaftlicher Nutzungsformen zu ermöglichen.

This work has been digitized and published in 2013 by Verlag Zeitschrift für Naturforschung in cooperation with the Max Planck Society for the Advancement of Science under a Creative Commons Attribution-NoDerivs 3.0 Germany License.

On 01.01.2015 it is planned to change the License Conditions (the removal of the Creative Commons License condition "no derivative works"). This is to allow reuse in the area of future scientific usage.

Table 1 (continued)

$M_{02}^{12} = -\frac{\eta\sqrt{2}}{\sqrt{5}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \quad M_{00}^{12} = 0;$	$M_{20}^{23} = \frac{\eta}{B\sqrt{10}} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \quad M_{2-2}^{23} = 0;$
$M_{02}^{13} = -\frac{\sqrt{6}\eta}{\sqrt{5}B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right);$	$M_{00}^{22} = \frac{3}{B^2} + \frac{\eta^2}{B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$
$M_{00}^{13} = \frac{-2\eta^2}{5B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right);$	$M_{02}^{23} = \frac{-\eta}{\sqrt{2}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$
$M_{22}^{22} = \frac{\eta^2}{2B^2} + \frac{(\eta^2+6)}{2B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$	$M_{22}^{23} = \frac{\eta^2}{2B^2} + \frac{\eta^2+6}{2B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$
$M_{20}^{22} = \frac{\eta\sqrt{6}}{2B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right);$	$M_{20}^{33} = \frac{-\eta\sqrt{3}}{\sqrt{10}B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right);$
$M_{2-2}^{22} = \frac{\eta^2}{2B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right);$	$M_{2-2}^{33} = \frac{\eta^2}{2B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right);$
$M_{22}^{23} = \frac{\sqrt{3}}{B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$	$M_{00}^{33} = \frac{4\eta^2+15}{5B^2} + \frac{\eta^2}{5B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$
Everywhere above $B^2 = (\eta^2 + 3)$ .	

the results are presented in Table 1. The sum over  $k'$  and  $q'$  in (3) is restricted by Eqs. (14) and (16) in [1].

We thank Dr. Francis P. Temme of the Department of Chemistry, Queen's University, Kingston, Ontario, Canada for a private communication.

This work is funded by a grant from the Natural Sciences and Engineering Research Committee of Canada (NSERC).

[1] M. S. Krishnan and B. C. Sanctuary, Z. Naturforsch. **41a**, 353 (1986).

## Errata

F. Winterberg, Relativistic Electron-Positron Gamma Ray Laser, Z. Naturforsch. **41a**, 1005–1008 (1986).

Due to a misprint in the typewritten manuscript the following corrections have to be made:

1. Equation (3) must read  $v_\perp^2/c^2 \cong I/\gamma I_A$  and Eq. (3a)  $v_\perp^2/c^2 \cong (I/\gamma I_A) \sqrt{1 - v_\perp^2/c^2}$ .

F. Winterberg, A Crucial Test for Einstein's Special Theory of Relativity Against the Lorentz-Poincaré Ether Theory of Relativity, Z. Naturforsch. **41a**, 1261–1266 (1986).

The following corrections have to be made:

1. At the end of the sentence following Eq. (1) it must read  $I/r > \sqrt{E/\sigma} \cong 10$ .
2. Equation (2) must read  $\operatorname{tg} \psi = \gamma \operatorname{tg} \varphi$ .
3. In Eq. (10) replace  $\omega_2$  with  $\omega_1$ .
4. Equation (8) must read  $\alpha(t) = A \sin(2\omega t + 2\delta)$ .
5. In Eq. (18) replace  $\sin(2\omega t - \pi/2)$  with  $\sin(2\omega t - \pi)$ .