

Evolution of Spin Density Matrix in Pure NQR

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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 η , will lead to incorrect results.

In this note, as in [1] the Hamiltonian

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

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

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

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

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

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Table 1.

$M_{11}^{11} = \frac{2(2\eta^2+3)}{5B^2} + \frac{(\eta^2+9)}{5B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$	
$M_{11}^{12} = \frac{3}{\sqrt{5}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$	
$M_{11}^{13} = \frac{\sqrt{3}}{5\sqrt{2}B^2} \left[(2-\eta^2) + (\eta^2-6) \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right];$	
$M_{1-1}^{11} = \frac{6\eta}{5B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right);$	
$M_{1-1}^{12} = \frac{\eta}{\sqrt{5}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$	
$M_{1-1}^{13} = \frac{\sqrt{6}\eta}{10B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right);$	
$M_{13}^{13} = \frac{-3\eta}{\sqrt{10}B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right);$	
$M_{1-3}^{13} = \frac{\eta^2}{\sqrt{10}B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right);$	
$M_{11}^{22} = \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$	$M_{11}^{23} = \frac{\sqrt{6}}{\sqrt{5}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$
$M_{1-1}^{22} = 0;$	$M_{1-1}^{23} = \frac{\sqrt{3}\eta}{\sqrt{10}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$
$M_{13}^{23} = -\frac{\eta}{\sqrt{2}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$	$M_{1-3}^{23} = 0;$
$M_{11}^{33} = \frac{(7\eta^2+18)}{10B^2} + \frac{3(\eta^2+4)}{10B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$	
$M_{1-1}^{33} = \frac{-6\eta}{5B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right);$	
$M_{13}^{33} = \frac{\sqrt{3}\eta}{\sqrt{5}B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right);$	
$M_{1-3}^{33} = \frac{\sqrt{3}\eta^2}{2\sqrt{5}B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right) \right);$	
$M_{33}^{33} = \frac{(\eta^2+6)}{2B^2} + \frac{\eta^2}{2B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$	$M_{3-3}^{33} = 0;$
$M_{00}^{33} = 0;$	$M_{00}^{10} = \frac{\eta^2+15}{5B^2} + \frac{4\eta^2}{5B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);$

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Table 1 (continued)

$$\begin{aligned}
M_{0\frac{1}{2}}^{1\frac{1}{2}} &= -\frac{\eta\sqrt{2}}{\sqrt{5}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); & M_{00}^{1\frac{1}{2}} &= 0; \\
M_{0\frac{1}{2}}^{1\frac{3}{2}} &= -\frac{\sqrt{6}\eta}{\sqrt{5}B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right); \\
M_{00}^{1\frac{3}{2}} &= \frac{-2\eta^2}{5B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right); \\
M_{\frac{1}{2}\frac{1}{2}}^{2\frac{1}{2}} &= \frac{\eta^2}{2B^2} + \frac{(\eta^2+6)}{2B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \\
M_{\frac{1}{2}\frac{1}{2}}^{2\frac{3}{2}} &= \frac{\eta\sqrt{6}}{2B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right); \\
M_{\frac{1}{2}-\frac{1}{2}}^{2\frac{1}{2}} &= \frac{\eta^2}{2B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right); \\
M_{\frac{1}{2}-\frac{1}{2}}^{2\frac{3}{2}} &= \frac{\sqrt{3}}{B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right);
\end{aligned}$$

$$\begin{aligned}
M_{\frac{3}{2}\frac{3}{2}}^{2\frac{3}{2}} &= \frac{\eta}{B\sqrt{10}} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); & M_{\frac{3}{2}-\frac{3}{2}}^{2\frac{3}{2}} &= 0; \\
M_{00}^{2\frac{1}{2}} &= \frac{3}{B^2} + \frac{\eta^2}{B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \\
M_{0\frac{1}{2}}^{2\frac{3}{2}} &= \frac{-\eta}{\sqrt{2}B} \sin\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \\
M_{\frac{1}{2}\frac{1}{2}}^{2\frac{3}{2}} &= \frac{\eta^2}{2B^2} + \frac{\eta^2+6}{2B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \\
M_{\frac{1}{2}\frac{1}{2}}^{3\frac{3}{2}} &= \frac{-\eta\sqrt{3}}{\sqrt{10}B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right); \\
M_{\frac{1}{2}-\frac{1}{2}}^{3\frac{3}{2}} &= \frac{\eta^2}{2B^2} \left(1 - \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right)\right); \\
M_{00}^{3\frac{3}{2}} &= \frac{4\eta^2+15}{5B^2} + \frac{\eta^2}{5B^2} \cos\left(\frac{B\tilde{Q}t}{\sqrt{3}}\right); \\
\text{Everywhere above } B^2 &= (\eta^2+3).
\end{aligned}$$

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

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[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 $l/r > \sqrt{E/\sigma} \cong 10$.
2. Equation (2) must read $\tan \psi = \gamma \tan \varphi$.
3. In Eq. (10) replace ω_2 with ω_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 $\sin(2\omega t - \pi)$.