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 $\frac{3}{2}$ 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 $\frac{3}{2}$ 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

$$
H_{\text{asym}} = \frac{e^2 Q q}{4I(2I - 1)} \left( \frac{1}{2} I_x^2 - I_z^2 + \frac{\eta}{2} (I_x^2 + I_y^2) \right)
$$

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

$$
\sigma(t) = \frac{1}{2I + 1} \sum_{k, q} \sum_{\nu, \pi} \sigma^{(k)q}(I) \Phi^{(k)q}_q(t)
$$

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

$$
\Phi^{(k)q}_q(t) = \sum_{k', q'} M^{k'q'}_{kq}(0) \Phi^{(k')q'}(0) .
$$

The matrix elements $M^{k'q'}_{kq}(t)$ 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 $\frac{3}{2}$ in NQR.

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

$$
M^{k'q'}_{kq} = (-1)^{k+k'} M^{k'q'}_{-kq} = (-1)^{k+k'} M^{k'q'}_{qq}
$$

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**Table 1.**

| $M_{11}$ | $M_{11} = \frac{2(2\eta^2 + 3) + (\eta^2 + 9)}{5B^2} \cos \left( \frac{B\hat{Q}t}{\sqrt{3}} \right)$ |
| $M_{11}$ | $M_{11} = \frac{3}{\sqrt{5}B} \sin \left( \frac{B\hat{Q}t}{\sqrt{3}} \right)$ |
| $M_{11}$ | $M_{11} = \frac{1}{\sqrt{5}B} \sin \left( \frac{B\hat{Q}t}{\sqrt{3}} \right)$ |
| $M_{11}$ | $M_{11} = \frac{1}{\sqrt{5}B} \sin \left( \frac{B\hat{Q}t}{\sqrt{3}} \right)$ |
| $M_{11}$ | $M_{11} = \frac{\eta}{\sqrt{5}B} \sin \left( \frac{B\hat{Q}t}{\sqrt{3}} \right)$ |
| $M_{11}$ | $M_{11} = \frac{\sqrt{3} \eta}{10B^2} \left( 1 - \cos \left( \frac{B\hat{Q}t}{\sqrt{3}} \right) \right)$ |
| $M_{11}$ | $M_{11} = \frac{\sqrt{3} \eta}{10B^2} \left( 1 - \cos \left( \frac{B\hat{Q}t}{\sqrt{3}} \right) \right)$ |
| $M_{11}$ | $M_{11} = \frac{(\eta^2 + 6)}{2\sqrt{5}B^2} \left( 1 - \cos \left( \frac{B\hat{Q}t}{\sqrt{3}} \right) \right)$ |
| $M_{11}$ | $M_{11} = \frac{(\eta^2 + 6)}{2\sqrt{5}B^2} \left( 1 - \cos \left( \frac{B\hat{Q}t}{\sqrt{3}} \right) \right)$ |
| $M_{11}$ | $M_{11} = \frac{(\eta^2 + 6)}{2\sqrt{5}B^2} \left( 1 - \cos \left( \frac{B\hat{Q}t}{\sqrt{3}} \right) \right)$ |

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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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Errata


Due to a misprint in the typewritten manuscript the following corrections have to be made:
1. Equation (3) must read $v/\gamma c^2 \approx l/\gamma I_a$ and Eq. (3a) $v/\gamma c^2 \approx (l/\gamma I_a) \sqrt{1 - v^2/c^2}$.


The following corrections have to be made:
1. At the end of the sentence following Eq. (1) it must read $l/r > \sqrt{E/\sigma} \geq 10$.
2. Equation (2) must read $\tan \psi = \gamma \tan \phi$.
3. In Eq. (10) replace $\omega_2$ with $\omega_1$.
4. Equation (8) must read $x(t) = A \sin (2 \omega t + 2 \delta)$.
5. In Eq. (18) replace $\sin (2 \omega t - \pi/2)$ with $\sin (2 \omega t - \pi)$.