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

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

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

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

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

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

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

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

Table 1.

$$M_{11}^{11} = \frac{2(2\eta^2+3)}{5B^2} + \frac{(\eta^2+9)}{5B^2} \cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

$$M_{11}^{12} = \frac{3}{\sqrt{5}B} \sin\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

$$M_{11}^{13} = \frac{\sqrt{3}}{5\sqrt{2}B^2} \left[(2-\eta^2) + (\eta^2-6)\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right];$$

$$M_{1-1}^{11} = \frac{6\eta}{5B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M_{1-1}^{12} = \frac{\eta}{\sqrt{5}B} \sin\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

$$M_{1-1}^{13} = \frac{\sqrt{6}\,\eta}{10B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M_{13}^{13} = \frac{-3\eta}{\sqrt{10}B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M_{1-3}^{13} = \frac{\eta^2}{\sqrt{10}B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M_{11}^{22} = \cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right); \quad M_{11}^{23} = \frac{\sqrt{6}}{\sqrt{5}B} \sin\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

$$M_{1-1}^{22} = 0; \quad M_{1-1}^{23} = \frac{\sqrt{3}\,\eta}{\sqrt{10}B} \sin\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

$$M_{13}^{23} = -\frac{\eta}{\sqrt{2}B} \sin\left(\frac{B\bar{Q}t}{\sqrt{3}}\right); \quad M_{1-3}^{23} = 0;$$

$$M_{11}^{33} = \frac{(7\eta^2+18)}{10B^2} + \frac{3(\eta^2+4)}{10B^2} \cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

$$M_{1-1}^{33} = \frac{-6\eta}{5B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M_{13}^{33} = \frac{\sqrt{3}\,\eta}{\sqrt{5}B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M_{1-3}^{33} = \frac{\sqrt{3}\,\eta^2}{2\sqrt{5}B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M_{33}^{33} = \frac{(\eta^2+6)}{2B^2} + \frac{\eta^2}{2B^2} \cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right); \quad M_{3-3}^{33} = 0;$$

$$M_{00}^{23} = 0; \quad M_{00}^{11} = \frac{\eta^2+15}{5B^2} + \frac{4\eta^2}{5B^2} \cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

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Table 1 (continued)

$$M^{1\,2}_{0\,2} = -\frac{\eta\sqrt{2}}{\sqrt{5}\,B}\sin\left(\frac{B\bar{Q}t}{\sqrt{3}}\right); \qquad M^{1\,2}_{0\,0} = 0;$$

$$M^{1\,3}_{0\,2} = -\frac{\sqrt{6}\,\eta}{\sqrt{5}\,B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M^{1\,3}_{0\,0} = \frac{-2\eta^2}{5B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M^{2\,2}_{2\,2} = \frac{\eta^2}{2B^2}+\frac{(\eta^2+6)}{2B^2}\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

$$M^{2\,2}_{2\,0} = \frac{\eta\sqrt{6}}{2B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M^{2\,2}_{2\,-2} = \frac{\eta^2}{2B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M^{2\,3}_{2\,2} = \frac{\sqrt{3}}{B}\sin\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

$$M^{2\,3}_{2\,0} = \frac{\eta}{B\sqrt{10}}\sin\left(\frac{B\bar{Q}t}{\sqrt{3}}\right); \qquad M^{2\,3}_{2\,-2} = 0;$$

$$M^{2\,2}_{0\,0} = \frac{3}{B^2}+\frac{\eta^2}{B^2}\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

$$M^{2\,3}_{0\,2} = \frac{-\eta}{\sqrt{2}\,B}\sin\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

$$M^{3\,3}_{2\,2} = \frac{\eta^2}{2B^2}+\frac{\eta^2+6}{2B^2}\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

$$M^{3\,3}_{2\,0} = \frac{-\eta\sqrt{3}}{\sqrt{10}\,B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M^{3\,3}_{2\,-2} = \frac{\eta^2}{2B^2}\left(1-\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right)\right);$$

$$M^{3\,3}_{0\,0} = \frac{4\eta^2+15}{5B^2}+\frac{\eta^2}{5B^2}\cos\left(\frac{B\bar{Q}t}{\sqrt{3}}\right);$$

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].

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