

Precession Equation of a Spinning Particle in Nonuniform Fields

U. FANO

National Bureau of Standards, Washington, D. C.

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The general equation governing the changes of orientation of a spinning particle is expressed in a compact tensorial form which represents an extension of the vector equation of Larmor precession. The time derivative of each component of a mean multipole moment of the particle is a linear combination of the multipole moments of all orders, subject to selection rules which express the interesting features of the motion.

THE orientation of a spinning particle changes under the influence of the torques exerted by external fields on the particle's multipole moments of various orders. The simplest example of such a change is the Larmor precession of the particle's magnetic moment $\langle \mathbf{u} \rangle$ about the direction of a uniform magnetic field \mathbf{H} ; this precession obeys the equation

$$d\langle \mathbf{u} \rangle / dt = -\gamma \mathbf{H} \times \langle \mathbf{u} \rangle, \quad (1)$$

where γ indicates the gyromagnetic ratio of the particle and $\langle \mathbf{u} \rangle$ the quantum-mechanical expectation value (the "mean") of its dipole magnetic moment. The next more complicated example occurs when a nucleus with spin of ≥ 1 is subjected to electric field gradients, say, in a crystal lattice. The changes of orientation of a nucleus are detectable, for example, when they occur in the interval between two γ -ray emissions, because they affect the angular correlation of these radiations. Changes of orientation of molecules as they traverse electric or magnetic lenses with complex field configurations are also detectable.

We wish to consider here the changes of orientation of a particle under the influence of arbitrary nonuniform fields. However, linear dependence of the effects on the field strengths will be assumed, thereby disregarding possible deformations of the particle by the fields.

Since the orientation of a particle is represented, in general, by a density matrix, its variation in the course of time is represented by the relevant time-dependent Schrödinger equation for this matrix. The number of elements of the orientation density matrix for a spin- j particle, namely $(2j+1)^2$, is rather large except for the elementary case of spin $\frac{1}{2}$. Therefore, it may take some effort to visualize what changes of orientation will occur in any specific case and how they will relate to the field strengths and geometry and to the multipole moments of the particle.

Experimental and theoretical studies have been made of nuclear changes of orientation under the influence of torques acting on their magnetic dipole and electric quadrupole moments, almost exclusively for axially symmetric fields.¹ To proceed further and to extend the

studies to particles other than nuclei, one should identify geometrical and dynamical situations that are nontrivial, amenable to experimental investigation and capable of providing new information either on the multipole moments of particles or on the fields to which they are subjected. Even though no specific suggestion is offered to this end, it might perhaps be of help to present here a tensorial form of the Schrödinger equation for the changes of orientation. This form constitutes a direct generalization of the vector equation (1) and displays a few symmetries and other general properties.

Consider a particle whose angular momentum eigenstates are classified by a total angular momentum quantum number j , a magnetic quantum number m and additional quantum numbers, if any, indicated by α . Its state of orientation can be represented by density matrix elements $\langle \alpha jm | \rho | \alpha jm' \rangle$ diagonal in α and j . The general form of the Schrödinger equation for a density matrix is

$$d\rho/dt = -i\hbar^{-1}(\mathcal{H}\rho - \rho\mathcal{H}). \quad (2)$$

The matrix elements of \mathcal{H} and ρ which are of interest for our problem, namely, those diagonal in α and j , can be replaced by a linear substitution with standard tensorial sets² of parameters, i.e., with new quantities that transform under coordinate rotations like the complex conjugates of spherical harmonics Y_{kq}^* . The substitution, Eq. (18.1) of FR,² is for the density matrix³

$$\rho^{(k)}_q = \sum_{m,m'=j}^j (-1)^{j-m'} \times (jjkq | jm, j-m') \langle \alpha jm | \rho | \alpha jm' \rangle, \quad (3)$$

for

$$0 \leq k \leq 2j, \quad -k \leq q \leq k,$$

where $(jjkq | jm, j-m')$ is a Wigner coefficient. Each $\rho^{(k)}_q$ is proportional to the complex conjugate of the corresponding mean 2^k -pole moment component of the

systems without axial symmetry has been done by E. Matthias, W. Schneider, and R. M. Steffen, *Phys. Rev.* **125**, 161 (1962); *Arkiv Fysik* **24**, 97 (1963).

² U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic Press Inc., New York, 1959), to be referred as FR.

³ Since only matrix elements diagonal in (α, j) are involved here and these indices need not be shown explicitly, the symbol $[\langle \alpha j | \rho | \alpha j \rangle]^{(k)}_q$ of FR can be replaced here by the simpler notation $\rho^{(k)}_q$.

¹ See, e.g., S. Devons and L. J. B. Goldfarb, *Encyclopedia of Physics*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 42, pp. 513 ff.; V. Gillet, *Nucl. Phys.* **20**, 561 (1960). I thank Dr. Gillet for a friendly discussion, comments and advice on the subject of the present paper. Analytical and numerical work on

particle, $\langle \mathfrak{M}^{[k]}_q \rangle^*$ (FR, p. 105). Thus the state of orientation of the particle is characterized by parameters with immediate geometric significance.

The Hamiltonian of the particle orientation consists of a sum of terms representing multipole interactions of various orders, namely, $\mathcal{H} = \sum_{k=1}^{2j} \sum_q \mathfrak{M}^{[k]}_q \mathfrak{A}^{(k)}_q$. Here $\mathfrak{M}^{[k]}_q$ indicates the q th component of the 2^k -pole moment operator of the particle and $\mathfrak{A}^{(k)}_q$ is the corresponding component of an irreducible standard tensor constructed with space derivatives of order $k-1$ of the electric or magnetic field.⁴ Each matrix element of a multipole moment operator is, according to the Wigner-Eckart theorem (FR, p. 79), the product of a "reduced" matrix element independent of orientation and of a Wigner coefficient, $(\alpha jm | \mathfrak{M}^{[k]}_q | \alpha j m') = (-1)^{j-m'} \times (2k+1)^{-1/2} (\alpha j || M^{[k]} || \alpha j) (jm, j-m' | j j k q)$. Therefore we may define, in analogy to (3), multipole parameters of the interaction

$$\begin{aligned} \Omega^{(k)}_q &= \hbar^{-1} \sum_{m, m'} (-1)^{j-m'} \\ &\quad \times (j j k q | j m, j-m') (\alpha jm | \mathcal{H} | \alpha j m') \quad (4) \\ &= \hbar^{-1} (2k+1)^{-1/2} (\alpha j || M^{[k]} || \alpha j) \mathfrak{A}^{(k)}_q. \end{aligned}$$

Inclusion of the factor \hbar^{-1} gives $\Omega^{(k)}_q$ the dimensions of a frequency. The factor $\hbar^{-1} (2k+1)^{-1/2} (\alpha j || M^{[k]} || \alpha j)$ is a generalization of the gyromagnetic ratio.

With these notations the calculation of the matrix product $\mathcal{H}\rho$ in (2) reduces to a recoupling operation of Racah algebra, which yields, according to (18.18) of FR,

$$\begin{aligned} \hbar^{-1} (\mathcal{H}\rho)^{(k)}_q &= \sum_{k_1 k_2} (-1)^{2j+k} [(2k_1+1)(2k_2+1)]^{1/2} \\ &\quad \times \bar{W} \begin{pmatrix} k_1 k_2 k \\ j j j \end{pmatrix} [\Omega^{(k_1)} \times \rho^{(k_2)}]^{(k)}_q. \quad (5) \end{aligned}$$

Here the $(\mathcal{H}\rho)^{(k)}_q$ have been obtained from the matrix elements $(\alpha jm | \mathcal{H}\rho | \alpha j m')$ by the substitution (3), the Racah \bar{W} coefficient is the same as the Wigner $6j$ symbol with the same indices⁵ and

$$[\Omega^{(k_1)} \times \rho^{(k_2)}]^{(k)}_q = \sum_{q_1 q_2} (k_1 k_2 k q | k_1 q_1 k_2 q_2) \Omega^{(k_1)}_{q_1} \rho^{(k_2)}_{q_2} \quad (6)$$

is a component of the irreducible product of degree k of the tensorial sets $\Omega^{(k_1)}$ and $\rho^{(k_2)}$. [The product (6) exists only for values of k_1 , k_2 and k that fulfill the "triangular conditions" $|k_1 - k_2| \leq k \leq k_1 + k_2$ etc.] Calculation of the other matrix product in (2), namely $\hbar^{-1} \rho \mathcal{H}$, yields the same result (5) except for permutation of the factors of the irreducible product. This permutation has the effect of multiplying the result by $(-1)^{k_1+k_2-k}$, owing to the symmetry properties of the

⁴ As is well known, the multipole interactions are electric or magnetic for even or odd values of k , respectively, because matrix elements diagonal in (α, j) vanish for operators that are odd under inversion of space coordinates.

⁵ For an extensive table of the $6j$ symbols, which also provides the ordinary Wigner coefficients, see M. Rotenberg, R. Bivins, N. Metropolis, and John K. Wooten, Jr., *The 3-j and 6-j Symbols* (Technology Press, Cambridge, Massachusetts, 1959).

Wigner coefficients (see, e.g., p. 37 of FR). Therefore, application of the substitution (3) to the ordinary matrix representation of (2) yields the desired tensorial form of this equation

$$\begin{aligned} d\rho^{(k)}/dt &= -i \sum_{k_1 k_2} (-1)^{2j+k} [1 - (-1)^{k_1+k_2-k}] \\ &\quad \times [(2k_1+1)(2k_2+1)]^{1/2} \bar{W} \begin{pmatrix} k_1 k_2 k \\ j j j \end{pmatrix} [\Omega^{(k_1)} \times \rho^{(k_2)}]^{(k)}, \quad (7) \end{aligned}$$

where boldface letters indicate collectively entire sets of tensorial components with different indices q . Equation (7) displays explicitly which multipole parameters of the interaction, $\Omega^{(k_1)}$, are effective through coupling with given multipole parameters of the initial orientation, $\rho^{(k_2)}$, in bringing about time changes of that orientation.

A principal characteristic of (7) is the factor $1 - (-1)^{k_1+k_2-k}$ which vanishes unless k_1+k_2-k is odd, that is, unless $[\Omega^{(k_1)} \times \rho^{(k_2)}]^{(k)}$ is odd with respect to permutation of its factors. The oddness of the vector product $\mathbf{H} \times \langle \mathbf{u} \rangle$ in (1) is a special case of this rule; in fact the right-hand side of (1) is equivalent to the term of (7) that contains only vectors (tensorial sets of degree 1), i.e., to the term with $k_1=k_2=k=1$. The vector product $\mathbf{H} \times \langle \mathbf{u} \rangle$ represents a torque, which changes the direction of $\langle \mathbf{u} \rangle$ but leaves invariant its squared magnitude $|\langle \mathbf{u} \rangle|^2$. Similarly, the odd products on the right of (7) may be regarded as generalized torques which change the orientation parameters $\rho^{(k)}_q$ but leave invariant their aggregate square magnitude⁶

$$S = \sum_{k=1}^{2j} \sum_q |\rho^{(k)}_q|^2 = \sum_{k=1}^{2j} |\rho^{(k)}|^2. \quad (8)$$

The sum S is an index of the degree of orientation or of polarization of the particle state, since it vanishes only in the state of random orientation, in which $\rho^{(k)}_q = 0$ for $k \neq 0$. The various subsums $|\rho^{(k)}|^2$ represent different "kinds" of polarization, namely, dipole, quadrupole, . . . polarization, respectively, for $k=1, 2, \dots$ (see also FR, p. 105). Equation (7) does not preserve, in general, the magnitudes of the separate kinds of polarization, i.e., of the individual $|\rho^{(k)}|^2$.

Conservation of the separate $|\rho^{(k)}|^2$ occurs only in the case of uniform external fields in which $\Omega^{(k_1)} = 0$ for $k_1 > 1$ and consequently only terms with $k_2 = k$ fail to vanish on the right of (7). The equation represents then a simultaneous simple precession of all separate 2^k -pole sets of parameters $\rho^{(k)}$ about the direction of the uniform magnetic field with equal Larmor frequencies. In this case, but only in this case, the change of orientation of the spinning particle resembles the precession of a classical top whose shape parameters are constant.

⁶ The parameter $\rho^{(0)}_0 = (2j+1)^{-1/2} \text{Tr} \rho = (2j+1)^{1/2}$ is the same for all states and is constant in time according to (7), so that it need not be considered.

A milder restriction on the changes of orientation, corresponding to another subgroup of these motions, occurs when the electric field is uniform or vanishing but the magnetic field is arbitrary. In this case $\Omega^{(k_1)}$ vanishes for all even values of k_1 and only terms remain on the right of (7) for which k_2 and k have the same parity. The sets of electric and magnetic 2^k -pole parameters—with k even and odd, respectively—do not interact then and we have two separate invariants, instead of (8) alone, namely

$$S_{el} = \sum_{k \text{ even}} |\rho^{(k)}|^2 \quad \text{and} \quad S_{magn} = \sum_{k \text{ odd}} |\rho^{(k)}|^2. \quad (9)$$

Conversely, a nonuniform electric field in the absence of magnetic field causes only variations of the magnetic parameters (with odd k) proportional to the electric ones and variations of the electric parameters proportional to the magnetic ones. A simple example of this effect occurs when nuclei are initially "aligned" in a certain direction but not "polarized," i.e., when $\rho^{(k)}_q \neq 0$ only for k even and $q=0$; an electric field gradient yielding $\Omega^{(2)}_q \neq 0$ for $q \neq 0$ will then generate an orientation represented by $d\rho^{(1)}_q/dt$ and/or $d\rho^{(3)}_q/dt \neq 0$.

In the event of axial symmetry of all fields and field gradients, the coordinate axis is appropriately laid along the symmetry axis and all $\Omega^{(k_1)}_q$ with $q_1 \neq 0$ vanish. Equation (7) reduces then to terms that relate parameters $d\rho^{(k)}_q/dt$ to $\rho^{(k_2)}_{q_2}$ with $q_2 = q$. The original, nontensorial form (2) of the equation of motion is particularly simple here, because the magnitude of each matrix element ($\alpha jm | \rho | \alpha j m'$) is now constant and its phase varies like $\exp[i(E_m - E_{m'})t/\hbar]$, where the magnetic quantum numbers m are now constants of the motion and E_m is an energy eigenvalue. In this event, each $\rho^{(k)}_q$ with $q \neq 0$ is a linear combination of different $(m | \rho | m')$ with different $E_m - E_{m'}$ though equal $m - m'$ and therefore oscillates in magnitude in the course of time; however the $\sum_k |\rho^{(k)}_q|^2$ is constant for each value of q .

Example: spin 1

We write here, for purposes of illustration, the equation of motion (7) for $j=1$ with the appropriate numerical values of the Racah and Wigner coefficients and in terms of ordinary Cartesian components of the electric and magnetic fields \mathbf{E} and \mathbf{H} and of their derivatives. The elements of the standard sets of parameters $\rho^{(k)}$ are related to sets with other normalizations in accordance with FR, pp. 24, 25, and 105.

The intrinsic magnetic moment μ of the particle is defined as usual as the mean value of μ_z in the state ($j=1, m=1$) and the quadrupole moment Q as the mean value of $3z^2 - r^2$ times the density of positive charge in the same state. One finds then

$$\begin{aligned} \Omega^{(1)}_1 &= -\Omega^{(1)}_{-1}^* = \hbar^{-1}\mu(H_x - iH_y), \\ \Omega^{(1)}_0 &= -\sqrt{2}\hbar^{-1}\mu H_z, \\ \Omega^{(2)}_2 &= \Omega^{(2)}_{-2}^* = -\frac{1}{2}\hbar^{-1}Q\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)(E_x - iE_y), \\ \Omega^{(2)}_1 &= -\Omega^{(2)}_{-1}^* = \frac{1}{4}\hbar^{-1}Q \\ &\quad \times \left[\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)E_z + \frac{\partial}{\partial z}(E_x - iE_y) \right], \\ \Omega^{(2)}_0 &= -\left(\frac{3}{8}\right)^{1/2} \hbar^{-1}Q \frac{\partial E_z}{\partial z}, \end{aligned} \quad (10)$$

and

$$\begin{aligned} d\rho^{(1)}_1/dt &= i\left\{ \sqrt{\frac{1}{2}}(\Omega^{(1)}_1\rho^{(1)}_0 - \Omega^{(1)}_0\rho^{(1)}_1) \right. \\ &\quad \left. - (\Omega^{(2)}_2\rho^{(2)}_{-1} - \Omega^{(2)}_{-1}\rho^{(2)}_2) \right. \\ &\quad \left. + \sqrt{\frac{3}{2}}(\Omega^{(2)}_1\rho^{(2)}_0 - \Omega^{(2)}_0\rho^{(2)}_1) \right\}, \\ d\rho^{(1)}_0/dt &= i\left\{ \sqrt{\frac{1}{2}}(\Omega^{(1)}_1\rho^{(1)}_{-1} - \Omega^{(1)}_{-1}\rho^{(1)}_1) \right. \\ &\quad \left. - \sqrt{2}(\Omega^{(2)}_2\rho^{(2)}_{-2} - \Omega^{(2)}_{-2}\rho^{(2)}_2) \right. \\ &\quad \left. + \sqrt{\frac{1}{2}}(\Omega^{(2)}_1\rho^{(2)}_{-1} - \Omega^{(2)}_{-1}\rho^{(2)}_1) \right\}, \quad (11) \\ d\rho^{(2)}_2/dt &= i\left\{ (\Omega^{(1)}_1\rho^{(2)}_1 - \Omega^{(2)}_1\rho^{(1)}_1) \right. \\ &\quad \left. - \sqrt{2}(\Omega^{(1)}_0\rho^{(2)}_2 - \Omega^{(2)}_2\rho^{(1)}_0) \right\}, \\ d\rho^{(2)}_1/dt &= i\left\{ \sqrt{\frac{3}{2}}(\Omega^{(1)}_1\rho^{(2)}_0 - \Omega^{(2)}_0\rho^{(1)}_1) \right. \\ &\quad \left. - \sqrt{\frac{1}{2}}(\Omega^{(1)}_0\rho^{(2)}_1 - \Omega^{(2)}_1\rho^{(1)}_0) \right. \\ &\quad \left. - (\Omega^{(1)}_{-1}\rho^{(2)}_2 - \Omega^{(2)}_2\rho^{(1)}_{-1}) \right\}, \\ d\rho^{(2)}_0/dt &= i\sqrt{\frac{3}{2}}\left\{ \Omega^{(1)}_1\rho^{(2)}_{-1} - \Omega^{(2)}_{-1}\rho^{(1)}_1 \right. \\ &\quad \left. - \Omega^{(1)}_{-1}\rho^{(2)}_1 + \Omega^{(2)}_1\rho^{(1)}_{-1} \right\}. \end{aligned}$$

The equations with $q < 0$ are obtained from those with $q > 0$ by reversing the sign of all q and the sign in front of the braces. A form of (11) without any imaginary element is obtained by replacing the standard sets of parameters $\rho^{(1)}$ and $\rho^{(2)}$ with the corresponding "real standard" sets.⁷

⁷ U. Fano, J. Math. Phys. 1, 417 (1960).