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An NMR rotation operator disentanglement strategy for establishing properties of the Euler–Rodrigues parameters

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Abstract. A disentanglement of the rotation operator introduced by Santiago and Vaidya is used to prove the composition rule for the Euler–Rodrigues parameters in a representation-independent manner. It is also shown that one of the Santiago and Vaidya disentangling coefficients embodies the Darboux transformation of differential geometry, which is equivalent to stereographic projection of the Bloch sphere onto the complex plane.

Stuelpnagel (1964) has shown that no three-dimensional parametrization of the rotation group $SO(3)$ can be both global *and* non-singular. In the case of the Euler angles (α, β, γ), for example, this leads to well known singularities for defining a rotation (Hughes 1986), and in the Euler angle kinematic equations (Evans 1977). Not only that, the Euler angle kinematic equations are *nonlinear*. At the price of one redundant parameter, the four-dimensional Euler–Rodrigues (ER) parametrization offers, by comparison, a number of important advantages. Expressed in terms of the rotation axis, $\hat{\boldsymbol{n}}$, and the rotation angle, Φ, the ER parameters $\{\lambda, \boldsymbol{\Lambda}\} \equiv \{\cos\frac{\Phi}{2}, \hat{\boldsymbol{n}}\sin\frac{\Phi}{2}\}$ are the *only* parameters for which the group multiplication rule can be given in closed form (Altmann 1986) as a simple bilinear composition (*vide infra*). They are also the representation of smallest dimension which has such a bilinear composition rule, and consequently a *linear* kinematic equation (Shuster 1993, Stuelpnagel 1964).

Some years ago, Santiago and Vaidya (1976) showed how the matrix elements of the rotation operator could be evaluated in an extremely simple manner by using Baker–Campbell–Hausdorff (BCH) formulae for the exponentials of the generators of the $SU(2)$ group. For the case of a rotation axis/rotation angle $\{\Phi, \hat{\boldsymbol{n}}\}$ parametrization of the rotation operator $\mathcal{D} = \exp[-\mathrm{i}\Phi\hat{\boldsymbol{n}}\cdot\boldsymbol{I}]$, their disentanglement of $\mathcal{D}$ as $\mathcal{D} = \exp[A_+I_+]\exp[\ln(A_0)I_0]\exp[A_-I_-]$ introduced c-number disentangling coefficients $\{A_+(\Phi,\hat{\boldsymbol{n}}), A_0(\Phi,\hat{\boldsymbol{n}}), A_-(\Phi,\hat{\boldsymbol{n}})\}$ which considerably simplified the evaluation of the required matrix elements $\mathcal{D}^{(I)}_{mn}(\Phi,\hat{\boldsymbol{n}})$. However, it appears to have been overlooked that if these c-number disentangling coefficients are expressed in terms of the ER parameters $\{\lambda, \boldsymbol{\Lambda}\}$ as $\{A_+(\lambda,\boldsymbol{\Lambda}), A_0(\lambda,\boldsymbol{\Lambda}), A_-(\lambda,\boldsymbol{\Lambda})\}$, then the particular disentanglement technique employed by Santiago and Vaidya (1976) also provides a direct and simple route for establishing several important properties of the ER parameters. These properties include their composition rule, as we show in this comment, and their kinematic relations, as shown previously (Siminovitch 1995). The simplicity and linearity of these ER parameter

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relations have been used to some advantage in spin kinematics (Counsell *et al* 1985, Barbara 1986) and spacecraft attitude kinematics (Hughes 1986, Shuster 1993). Due to their simple composition rule, the ER parameters continue to play an increasingly important role in NMR, where composing rotations are indispensable in pulse sequence design (Levitt 1986), and in calculating the response to multipulse sequences (Barbara 1994, Lu *et al* 1996).

In the context of NMR, the present comment has two purposes. First, we take advantage of the Santiago and Vaidya (1976) disentanglement procedure to establish the ER parameter composition rule in a representation-independent manner. We believe that this provides the first quantum mechanical argument to establish the validity of the ER parameter composition rule for spins of arbitrary magnitude, I, without choosing a representation. Secondly, we note that the expression for the c-number coefficient $A_+ \equiv A_+(\lambda, \mathbf{\Lambda})$ in the Santiago and Vaidya (1976) disentanglement of the quantum mechanical rotation operator embodies transformations of two sets of coupled equations of motion. Both sets, one the Euler kinematical relations (Zhou *et al* 1993, 1994), and the other the Bloch equations, provide a *classical* description of spin kinematics. One of these transformations is the Darboux (1887) transformation of differential geometry (Eisenhart 1960, Melzak 1976) transforming the Frenet–Serret equations into the Riccati equation. Since the Frenet–Serret equations are formally identical to the Bloch equations in NMR (Lamb 1971), in a classical description of magnetization vector trajectories in NMR, the Darboux (1887) transformation is equivalent to stereographic projection of the Bloch sphere onto the complex plane (Corio 1966). The other is a transformation introduced by Zhou *et al* (1994), transforming the Euler kinematic equations of rigid body dynamics into the Riccati equation.

Using the ER parameters, a composition rule for the $SO(3)$ rotation matrices $\mathbf{R}(\lambda, \mathbf{\Lambda})$ can be defined. The compounding formula of Counsell *et al* (1985) for the product of two such consecutive three-dimensional rotations applied to a spin system takes the following standard form (rotation through an angle Φ_1 about $\hat{\boldsymbol{n}}_1$ followed by rotation through an angle Φ_2 about $\hat{\boldsymbol{n}}_2$):

$$\mathbf{R}_1(\lambda_1, \mathbf{\Lambda}_1)\mathbf{R}_2(\lambda_2, \mathbf{\Lambda}_2) = \mathbf{R}(\lambda, \mathbf{\Lambda}) \tag{1}$$

where

$$\lambda = \lambda_1\lambda_2 - \mathbf{\Lambda}_1 \cdot \mathbf{\Lambda}_2 \tag{2}$$

$$\lambda_i = \cos\left(\frac{\Phi_i}{2}\right) \qquad (i = 1, 2) \tag{3}$$

$$\mathbf{\Lambda}_i = \hat{\boldsymbol{n}}_i \sin\left(\frac{\Phi_i}{2}\right) \qquad (i = 1, 2) \tag{4}$$

$$\mathbf{\Lambda} = \lambda_2\mathbf{\Lambda}_1 + \lambda_1\mathbf{\Lambda}_2 - \mathbf{\Lambda}_1 \times \mathbf{\Lambda}_2. \tag{5}$$

This formula, originating from rigid body kinematics (Rodrigues 1840, Favro 1960, Altmann 1986), can be used for calculating the response to spin-$\frac{1}{2}$ composite pulses (Counsell *et al* 1985, Barbara 1994) as well as phase-alternating spin-1 composite pulses (Barbara 1986). From a classical point of view, the first purely *geometrical* approach to obtaining the resultant ER parameters $\{\lambda, \mathbf{\Lambda}\}$ for two consecutive rotations was taken by Rodrigues (1840), using the ER construction, and spherical trigonometry. An alternative geometrical derivation has recently been given by Sivardière (1994), based on the decomposition of a rotation into two reflections (Coxeter 1946, Misner *et al* 1973, Altmann 1986). Such a decomposition can be used to account for the presence of *half*-angles in the composition rule. An entirely different classical approach relies on the relationship between rotations and homographies (Cayley 1879, Biedenharn and Louck 1981). Under stereographic projection of the Bloch sphere onto the complex plane, rotations of points on the sphere correspond to homographic transformations $z \to z'$ of the complex plane. By parametrizing each homographic transformation via the ER parameters $\{\lambda, \mathbf{\Lambda}\}$ as

$$z' = \frac{(\lambda + \mathrm{i}\Lambda_z)z - (\Lambda_y - \mathrm{i}\Lambda_x)}{(\Lambda_y + \mathrm{i}\Lambda_x)z + (\lambda - \mathrm{i}\Lambda_z)} \tag{6}$$

a composition of two such homographies may also be used to obtain the ER parameter composition rule of equations (2)–(5) (Cayley 1879, Klein 1884).

Quantum mechanical proofs of this composition rule using the rotation axis/rotation angle $\{\Phi, \hat{\boldsymbol{n}}\}$ parametrization of the rotation operator have always relied on the spin-$\frac{1}{2}$ representation of the rotation group (Harter and dos Santos 1978, Counsell *et al* 1985). Since the composition rule relates only the angles and axes of the rotations, both of which are independent of the representation, a choice of the spin-$\frac{1}{2}$ representation is clearly sufficient (Counsell *et al* 1985). By the same token, it should not be necessary to choose *any* representation, which we now demonstrate by establishing the ER parameter composition rule of equations (2)–(5) in a representation-independent manner.

For this purpose, consider a set of operators $K_\pm \equiv K_x \pm \mathrm{i}K_y$ and $K_0 \equiv K_z$ which satisfy the usual commutation relations for the generators of the $SU(2)$ Lie algebra:

$$[K_-, K_+] = -2K_0 \tag{7}$$

$$[K_0, K_\pm] = \pm K_\pm. \tag{8}$$

Then the following normal-order decomposition formula for an exponential function of these generators can be derived (Santiago and Vaidya 1976, Truax 1985, Cheng and Fung 1988, Ban 1993):

$$\exp[a_+K_+ + a_0K_0 + a_-K_-] = \exp[A_+K_+]\exp[\ln(A_0)K_0]\exp[A_-K_-] \tag{9}$$

where

$$A_\pm = \frac{(a_\pm/f)\sinh f}{\cosh f - (a_0/2f)\sinh f} \tag{10}$$

$$A_0 = [\cosh f - (a_0/2f)\sinh f]^{-2} \tag{11}$$

$$f = [(a_0/2)^2 + a_-a_+]^{1/2}. \tag{12}$$

In order to generalize the decomposition formula of equation (9), the ordered product $G(n)$ of the exponential functions of the generators of the Lie algebra can be defined as follows (Ban 1993):

$$G(n) = \prod_{k=1}^{n} \exp[a_+(k)K_+ + a_0(k)K_0 + a_-(k)K_-] \tag{13}$$

where

$$\prod_{k=1}^{n} g(k) = g(n)g(n-1)\ldots g(2)g(1). \tag{14}$$

Using this notation, for arbitrary c-number functions $\{a_\pm\}$ and $\{a_0\}$, Ban (1993) has derived the following normal-order BCH formula for the ordered product $G(n)$:

$$\begin{aligned} G(n) &= \prod_{k=1}^{n} \exp[a_+(k)K_+ + a_0(k)K_0 + a_-(k)K_-] \\ &= \exp[A_+(n)K_+]\exp[\ln(A_0(n))K_0]\exp[A_-(n)K_-]. \end{aligned} \tag{15}$$

The c-number functions $\{A_\pm\}$ and $\{A_0\}$ are defined by Ban (1993) in terms of recursion formulae, of which the following formula for $A_+(n)$ will suffice for the purpose of illustration:

$$A_+(n) = \frac{(a_+/f(n))\sinh f(n) + \{\cosh f(n) + (a_0/2f(n))\sinh f(n)\}A_+(n-1)}{\cosh f(n) - (a_0/2f(n))\sinh f(n) + (a_-/f(n))\sinh f(n)A_+(n-1)} \tag{16}$$

where

$$A_+(0) = 0 \tag{17}$$

$$f(n) = [(a_0(n)/2)^2 + a_-(n)a_+(n)]^{1/2}. \tag{18}$$

The above formulae (equations (15)–(18)) for the ordered product $G(n)$ are not based on geometrical considerations, instead they were obtained by Ban (1993) by using induction and parameter differentiation (Wilcox 1967), and the commutation relations of equations (7) and (8). For a rotation first performed about the $\hat{\boldsymbol{n}}_1$ axis through the Φ_1 angle, followed by a second rotation about the $\hat{\boldsymbol{n}}_2$ axis through the Φ_2 angle, the operator $\mathcal{D}$ of the resultant rotation can be expressed in terms of an ordered product, $\mathcal{P}$, of rotation operators as

$$\mathcal{D} \equiv \exp[-\mathrm{i}\Phi\hat{\boldsymbol{n}}\cdot\boldsymbol{I}] = \exp[-\mathrm{i}\Phi_2\hat{\boldsymbol{n}}_2\cdot\boldsymbol{I}]\exp[-\mathrm{i}\Phi_1\hat{\boldsymbol{n}}_1\cdot\boldsymbol{I}] \equiv \mathcal{P}. \tag{19}$$

We now use the generalized BCH formula of equation (15) to show that the ER parameters $\{\lambda, \boldsymbol{\Lambda}\}$ of the resultant rotation can be expressed in terms of the ER parameters $\{\lambda_i, \boldsymbol{\Lambda}_i\}$ of the two consecutive rotations by the composition rule of equations (2)–(5). For this purpose, using the fact that the axis of rotation, $\hat{\boldsymbol{n}}$, is

$$\hat{\boldsymbol{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \tag{20}$$

the operator argument $-\mathrm{i}\Phi\hat{\boldsymbol{n}}\cdot\boldsymbol{I}$ of the rotation operator can be expressed in the notation of Ban (1993) as (Santiago and Vaidya 1976)

$$-\mathrm{i}\Phi\hat{\boldsymbol{n}}\cdot\boldsymbol{I} \equiv -\mathrm{i}\Phi(n_xI_x + n_yI_y + n_zI_z) = a_+I_+ + a_0I_0 + a_-I_- \tag{21}$$

where

$$a_\pm = -\mathrm{i}\Phi\sin\theta\frac{\mathrm{e}^{\mp\mathrm{i}\phi}}{2} \tag{22}$$

$$a_0 = -\mathrm{i}\Phi\cos\theta. \tag{23}$$

Using these expressions for the c-number functions $\{a_\pm\}$ and $\{a_0\}$, f of equation (12) is evaluated as (Santiago and Vaidya 1976)

$$f = \pm\mathrm{i}\frac{\Phi}{2} \tag{24}$$

so that the c-number functions $\{A_\pm\}$ and $\{A_0\}$ of equations (10) and (11) are defined in terms of the ER parameters $\{\lambda, \boldsymbol{\Lambda}\} \equiv \{\cos\frac{\Phi}{2}, \hat{\boldsymbol{n}}\sin\frac{\Phi}{2}\}$ as

$$A_\pm = -\mathrm{i}\frac{n_\mp\sin\frac{\Phi}{2}}{\left[\cos\frac{\Phi}{2} + n_z\sin\frac{\Phi}{2}\right]} \equiv -\mathrm{i}\frac{(\Lambda_x \mp \Lambda_y)}{\lambda + \mathrm{i}\Lambda_z} \tag{25}$$

$$A_0 = \left[\cos\frac{\Phi}{2} + n_z\sin\frac{\Phi}{2}\right]^{-2} \equiv [\lambda + \mathrm{i}\Lambda_z]^{-2} \tag{26}$$

where

$$n_\mp = n_x \mp \mathrm{i}n_y. \tag{27}$$

Using the notation of the generalized decomposition formula of equation (15), the ordered product, $\mathcal{P}$, of rotation operators on the RHS of equation (19) can be written as

$$\mathcal{P} = \exp[a_+(2)I_+ + a_0(2)I_0 + a_-(2)I_-]\exp[a_+(1)I_+ + a_0(1)I_0 + a_-(1)I_-] \tag{28}$$

$$= \exp[A_+(2)I_+]\exp[\ln(A_0(2))I_0]\exp[A_-(2)I_-]. \tag{29}$$

Using the recursion formula for $A_+(n)$ given in equation (16), we find

$$A_+(2) = \frac{-\mathrm{i}(\Lambda_{2x} - \mathrm{i}\Lambda_{2y}) + (\lambda_2 - \mathrm{i}\Lambda_{2z})A_+(1)}{(\lambda_2 + \mathrm{i}\Lambda_{2z}) - \mathrm{i}(\Lambda_{2x} + \mathrm{i}\Lambda_{2y})A_+(1)} \tag{30}$$

where

$$A_+(1) = -\mathrm{i}\frac{(\Lambda_{1x} - \mathrm{i}\Lambda_{1y})}{(\lambda_1 + \mathrm{i}\Lambda_{1z})}. \tag{31}$$

From equation (19), we must have $A_+ = A_+(2)$, so that from equations (25) and (30)

$$-\mathrm{i}\frac{(\Lambda_x - \mathrm{i}\Lambda_y)}{\lambda + \mathrm{i}\Lambda_z} = \frac{-\mathrm{i}(\Lambda_{2x} - \mathrm{i}\Lambda_{2y})(\lambda_1 + \mathrm{i}\Lambda_{1z}) + (\lambda_2 - \mathrm{i}\Lambda_{2z})(-\mathrm{i})(\Lambda_{1x} - \mathrm{i}\Lambda_{1y})}{(\lambda_2 + \mathrm{i}\Lambda_{2z})(\lambda_1 + \mathrm{i}\Lambda_{1z}) + (-\mathrm{i})(\Lambda_{2x} + \mathrm{i}\Lambda_{2y})(-\mathrm{i})(\Lambda_{1x} - \mathrm{i}\Lambda_{1y})} \tag{32}$$

or equivalently

$$\begin{aligned}\frac{\Lambda_y + \mathrm{i}\Lambda_x}{\lambda + \mathrm{i}\Lambda_z} = {} & \{[\lambda_2\Lambda_{1y} + \lambda_1\Lambda_{2y} + \Lambda_{1x}\Lambda_{2z} - \Lambda_{1z}\Lambda_{2x}] \\ & + \mathrm{i}[\lambda_2\Lambda_{1x} + \lambda_1\Lambda_{2x} + \Lambda_{1z}\Lambda_{2y} - \Lambda_{1y}\Lambda_{2z}]\} \\ & \times\{[\lambda_1\lambda_2 - \Lambda_{1x}\Lambda_{2x} - \Lambda_{1y}\Lambda_{2y} - \Lambda_{1z}\Lambda_{2z}] \\ & + \mathrm{i}[\lambda_2\Lambda_{1z} + \lambda_1\Lambda_{2z} + \Lambda_{1y}\Lambda_{2x} - \Lambda_{1x}\Lambda_{2y}]\}^{-1}.\end{aligned} \tag{33}$$

From a classical point of view, the composition of the two homographies corresponding to the rotations in the rotation operator product of equation (19) yields the following two equations (Cayley 1879, Klein 1884):

$$\begin{aligned}\Lambda_y + \mathrm{i}\Lambda_x = {} & [\lambda_2\Lambda_{1y} + \lambda_1\Lambda_{2y} + \Lambda_{1x}\Lambda_{2z} - \Lambda_{1z}\Lambda_{2x}] \\ & + \mathrm{i}[\lambda_2\Lambda_{1x} + \lambda_1\Lambda_{2x} + \Lambda_{1z}\Lambda_{2y} - \Lambda_{1y}\Lambda_{2z}]\end{aligned} \tag{34}$$

$$\begin{aligned}\lambda + \mathrm{i}\Lambda_z = {} & [\lambda_1\lambda_2 - \Lambda_{1x}\Lambda_{2x} - \Lambda_{1y}\Lambda_{2y} - \Lambda_{1z}\Lambda_{2z}] \\ & + \mathrm{i}[\lambda_2\Lambda_{1z} + \lambda_1\Lambda_{2z} + \Lambda_{1y}\Lambda_{2x} - \Lambda_{1x}\Lambda_{2y}].\end{aligned} \tag{35}$$

The quotient of these two equations is equation (33), and so we have recovered via the Santiago and Vaidya (1976) disentanglement procedure a relation which could have been obtained classically via stereographic projection. We return below to another connection between this disentanglement procedure and stereographic projection.

By using the relations of equation (33) and those obtained via the recursion relations for $A_-(n)$ and $A_0(n)$, as well as the fact that all the ER parameter sets $\{\lambda, \mathbf{\Lambda}\}$ define quaternions of unit norm (see equation (58) below), we find

$$\lambda = \pm\{\lambda_1\lambda_2 - \Lambda_{1x}\Lambda_{2x} - \Lambda_{1y}\Lambda_{2y} - \Lambda_{1z}\Lambda_{2z}\} \tag{36}$$

$$= \pm\{\lambda_1\lambda_2 - \mathbf{\Lambda}_1 \cdot \mathbf{\Lambda}_2\} \tag{37}$$

$$\Lambda_x = \pm\{\lambda_2\Lambda_{1x} + \lambda_1\Lambda_{2x} + \Lambda_{1z}\Lambda_{2y} - \Lambda_{1y}\Lambda_{2z}\} \tag{38}$$

$$= \pm\{\lambda_2\mathbf{\Lambda}_1 + \lambda_1\mathbf{\Lambda}_2 - (\mathbf{\Lambda}_1 \times \mathbf{\Lambda}_2)\}_x \tag{39}$$

$$\Lambda_y = \pm\{\lambda_2\Lambda_{1y} + \lambda_1\Lambda_{2y} + \Lambda_{1x}\Lambda_{2z} - \Lambda_{1z}\Lambda_{2x}\} \tag{40}$$

$$= \pm\{\lambda_2\mathbf{\Lambda}_1 + \lambda_1\mathbf{\Lambda}_2 - (\mathbf{\Lambda}_1 \times \mathbf{\Lambda}_2)\}_y \tag{41}$$

$$\Lambda_z = \pm\{\lambda_2\Lambda_{1z} + \lambda_1\Lambda_{2z} + \Lambda_{1y}\Lambda_{2x} - \Lambda_{1x}\Lambda_{2y}\} \tag{42}$$

$$= \pm\{\lambda_2\mathbf{\Lambda}_1 + \lambda_1\mathbf{\Lambda}_2 - (\mathbf{\Lambda}_1 \times \mathbf{\Lambda}_2)\}_z. \tag{43}$$

In terms of the resultant ER parameters $\{\lambda, \mathbf{\Lambda}\}$, equation (37) corresponds to that part of the ER parameter composition rule which defines λ (equation (2)), while equations (39), (41) and (43) are the respective x, y and z components of the *vector* equation defining $\mathbf{\Lambda}$ in the composition rule (equation (5)).

When commenting on this result, it should be noted that the proof itself depends *only* on the fact that the spin angular momentum operators, I_i, satisfy the commutation relations of equations (7) and (8) for the generators of the $SU(2)$ Lie algebra, and *not* on the spin magnitude, I, which is arbitrary. By establishing this result via the rotation operator in a representation-independent manner, we not only re-emphasize the spin-independent character of the ER composition rule, but we also avoid any pitfalls associated with choosing a particular representation. For example, by relying on the spin-$\frac{1}{2}$ algebra to establish Hamilton's equivalent of the ER composition rule, Harter and dos Santos (1978) have misleadingly attributed the *one-half* in the half-angles of the composition rule to the $\langle I_z \rangle = \frac{1}{2}$ value of angular momentum! In fact, this belies the fact that half-angles are an *essential feature* of the parametrization of rotations (Altmann 1986), as first demonstrated by Rodrigues (1840). The geometrical reason why *half*-angles appear in the composition rule is because a rotation through an angle, θ, about a given axis $\hat{\boldsymbol{n}}$ is equivalent to successive *reflections* in two planes that meet along this axis at the half-angle $\theta/2$ (Coxeter 1946, Misner *et al* 1973, Altmann 1986).

In the rotation operator approach (Popov 1959, Zhou *et al* 1993) for the description of spin dynamics in a time-varying magnetic field, the rotation operators may be parametrized in terms of the Euler angles α, β, γ (Zhou *et al* 1994), or in terms of the angle of rotation, Φ, about an axis $\hat{\boldsymbol{n}}$ (Siminovitch 1995). The corresponding rotation operators for each of these parametrizations are expressed as

$$\mathcal{D}(\alpha(t), \beta(t), \gamma(t)) = \exp[\mathrm{i}\gamma(t)I_z]\exp[\mathrm{i}\beta(t)I_y]\exp[\mathrm{i}\alpha(t)I_z] \tag{44}$$

$$\mathcal{D}(\Phi, \hat{\boldsymbol{n}}) = \exp[\mathrm{i}\Phi\hat{\boldsymbol{n}}\cdot\boldsymbol{I}] \tag{45}$$

using the *passive* convention (Bouten 1969), or as

$$\mathcal{D}(\alpha(t), \beta(t), \gamma(t)) = \exp[-\mathrm{i}\alpha(t)I_z]\exp[-\mathrm{i}\beta(t)I_y]\exp[-\mathrm{i}\gamma(t)I_z] \tag{46}$$

$$\mathcal{D}(\Phi, \hat{\boldsymbol{n}}) = \exp[-\mathrm{i}\Phi\hat{\boldsymbol{n}}\cdot\boldsymbol{I}] \tag{47}$$

using the *active* convention (Bouten 1969). By introducing the transformation

$$h = -\tan\frac{\beta}{2}\exp(\mathrm{i}\gamma) \tag{48}$$

Zhou *et al* (1994) showed that the *Euler kinematical relations* could be transformed into the Riccati equation for the variable h. The Riccati equation has played an extremely important role in NMR, reducing the integration of the *three* coupled first-order equations in the Bloch equations to a *single* first-order equation (Corio 1966). A further transformation of the Riccati equation to a linear second-order differential equation leads to a solution including the effects of radiation damping (Barbara 1992), and to exact analytical solutions for a small class of non-rectangular pulse shapes, including the hyberbolic secant pulse (Allen and Eberly 1975) and the exponentially shaped pulse (Campolieti and Sanctuary 1989, Keniry and Sanctuary 1990). These are the only other analytical solutions known besides that for a simple rectangular pulse.

On the other hand, substitution of the disentangled rotation operator, $\mathcal{D}(\Phi, \hat{\boldsymbol{n}})$, into the Schrödinger equation leads *directly* to the Riccati equation for the disentangling coefficient A_+ (Popov 1959, Cheng and Fung 1988)

$$\dot{A_+} = a_1{}' + a_2{}'A_+ - a_3{}'A_+^2 \tag{49}$$

where $a_j{}' \equiv -\mathrm{i}a_j$, and the coefficients a_j define the Hamiltonian $\mathcal{H}(t) = -\hbar\{a_1(t)I_+ + a_2(t)I_0 + a_3(t)I_-\}$. Therefore, by using the explicit form of the Santiago and Vaidya (1976) disentangling coefficient $A_+(\lambda, \mathbf{\Lambda})$ for the rotation operator in the passive convention used by Zhou *et al* (1994), and relations between the ER parameters $\{\lambda, \mathbf{\Lambda}\}$ and the Euler angles (α, β, γ), the transformation of equation (48) is directly and simply obtained by the conversion of $A_+ \equiv A_+(\lambda, \mathbf{\Lambda})$ to $A_+ \equiv A_+(\alpha, \beta, \gamma)$ as follows:

$$A_+ = \frac{\mathrm{i}(\Lambda_1 - \mathrm{i}\Lambda_2)}{\lambda - \mathrm{i}\Lambda_3} = \frac{\sin\frac{\beta}{2}\exp(-\mathrm{i}(\alpha-\gamma)/2)}{\cos\frac{\beta}{2}\exp(-\mathrm{i}(\alpha+\gamma)/2)} = \tan\frac{\beta}{2}\exp(\mathrm{i}\gamma). \tag{50}$$

(The change in sign between equation (48) and equation (50) is due to the difference between the Riccati equation of equation (49), and that used by Zhou *et al* (1994).) Similarly, consider the conversion of $A_+ \equiv A_+(\lambda, \mathbf{\Lambda})$ for the active form of the rotation operator to $A_+ \equiv A_+(M_x, M_y, M_z)$. By using the homomorphism between $SO(3)$ and $SU(2)$, the ER parametrization of the Rabi rotation matrix $\mathbf{R}(\lambda, \mathbf{\Lambda}) \in SO(3)$ may be obtained from $\mathbf{U}(\lambda, \mathbf{\Lambda}) \in SU(2)$ as

$$\mathbf{R}(\lambda, \mathbf{\Lambda}) = \begin{bmatrix} \lambda^2 + \Lambda_x^2 - \Lambda_y^2 - \Lambda_z^2 & 2(\Lambda_x\Lambda_y - \lambda\Lambda_z) & 2(\Lambda_z\Lambda_x + \lambda\Lambda_y) \\ 2(\Lambda_x\Lambda_y + \lambda\Lambda_z) & \lambda^2 - \Lambda_x^2 + \Lambda_y^2 - \Lambda_z^2 & 2(\Lambda_y\Lambda_z - \lambda\Lambda_x) \\ 2(\Lambda_z\Lambda_x - \lambda\Lambda_y) & 2(\Lambda_y\Lambda_z + \lambda\Lambda_x) & \lambda^2 - \Lambda_x^2 - \Lambda_y^2 + \Lambda_z^2 \end{bmatrix} \tag{51}$$

where

$$\mathbf{U}(\lambda, \mathbf{\Lambda}) = \begin{bmatrix} \lambda - \mathrm{i}\Lambda_z & -(\Lambda_y + \mathrm{i}\Lambda_x) \\ (\Lambda_y - \mathrm{i}\Lambda_x) & \lambda + \mathrm{i}\Lambda_z \end{bmatrix}. \tag{52}$$

The components of magnetization $\boldsymbol{M}(T) \equiv (M_x, M_y, M_z)$ at the end of a radiofrequency pulse of duration T can then be expressed in terms of the initial components $\boldsymbol{M}(0)$ and the elements of $\mathbf{R}(\lambda, \mathbf{\Lambda})$ as

$$\boldsymbol{M}(T) = \mathbf{R}\boldsymbol{M}(0). \tag{53}$$

Given typical initial conditions $\boldsymbol{M}(0) = (0, 0, 1)$ in NMR, the magnetization components can then be expressed in terms of the Rabi rotation matrix elements as

$$(M_x, M_y, M_z) = (\boldsymbol{R}_{13}, \boldsymbol{R}_{23}, \boldsymbol{R}_{33}). \tag{54}$$

By using the explicit form of $\mathbf{R}(\lambda, \mathbf{\Lambda})$ given in equation (51), we find

$$M_x = 2(\Lambda_x\Lambda_z + \lambda\Lambda_y) \tag{55}$$

$$M_y = 2(\Lambda_y\Lambda_z - \lambda\Lambda_x) \tag{56}$$

$$M_z = \lambda^2 + \Lambda_z^2 - (\Lambda_x^2 + \Lambda_y^2). \tag{57}$$

These relations, together with the normalization condition

$$\lambda^2 + \mathbf{\Lambda}^2 \equiv \lambda^2 + \Lambda_x^2 + \Lambda_y^2 + \Lambda_z^2 = 1 \tag{58}$$

may be used in the conversion of $A_+ \equiv A_+(\lambda, \mathbf{\Lambda})$ to $A_+ \equiv A_+(M_x, M_y, M_z)$. We find

$$A_+ = -\mathrm{i}\frac{(\Lambda_x - \mathrm{i}\Lambda_y)}{\lambda + \mathrm{i}\Lambda_z} = -\frac{1 - M_z}{M_x + \mathrm{i}M_y} = -\frac{1}{\sigma} \tag{59}$$

where σ is the parameter introduced by Darboux (1887) to transform the Frenet–Serret equations into the Riccati equation. By noting the analogy between the Frenet–Serret equations of differential geometry, and the Bloch equations in the absence of relaxation or radiation damping, Lamb (1971) introduced the analogue of the Darboux parameter, thereby reducing the Bloch equations into a single first-order Ricatti equation.

Starting with two of the classical descriptions of spin kinematics, one in the form of the Euler kinematical relations (Zhou *et al* 1993, 1994), and the other in the form of the more commonly used Bloch equations, a suitable transformation must be found in each case in order to reduce a set of coupled equations to a single first-order Riccati equation. Alternatively, as shown above, either of these transformations may be determined simply by re-expressing the Santiago and Vaidya (1976) disentangling coefficient $A_+(\lambda, \mathbf{\Lambda})$ as $A_+(\alpha, \beta, \gamma)$, or as $A_+(M_x, M_y, M_z)$, respectively.

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