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Matrix Treatment of Nuclear Induction*

E. T. JAYNES
Department of Physics and W. W. Hansen Laboratories of Physics, Stanford University, Stanford, California
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By use of matrix notation, solutions of the Bloch equations may be kept in simple, manageable form even in the case of applied fields that are complicated functions of time. Effects that from the usual standpoint are grossly nonlinear appear as linear relations between matrices, of the same form that one encounters in simple radioactive decay problems. A general property of transients in the case of an arbitrary repetitive applied signal is established, and a formalism is set up in terms of which a large class of special problems may be solved.

I. INTRODUCTION

THE following is an exposition of a method of finding solutions of the Bloch equations[1] making use of matrix theory. It has the advantage that formal solutions are derived in matrix form, with details worked out only at the end of a calculation, the desired result appearing typically as one element of a certain matrix. Although it is undoubtedly true that no solutions can be found by matrix methods which could not have been found without them, the saving of labor due to the condensed notation makes a wider range of calculations feasible. For example, in the companion paper[2] it is shown that Hahn's results[3] on the theory of spin echoes can be rederived in a very simple way and extended to more complicated situations; at the same time certain finer details such as the exact timing and shape of spin-echo signals are readily accounted for. In addition, the matrices correspond to simple geometrical operations so that a great deal of physical information can be read off directly from a matrix expression.

II. GENERAL FORMALISM

The Bloch equation[1] of motion of the nuclear magnetization M due to a magnetic field H will be taken in the form,

$$\frac{\partial \mathbf{M}}{\partial t}+\frac{\mathbf{M}-\chi\mathbf{H}}{T}+\gamma(\mathbf{H}\times\mathbf{M})=0, \tag{1}$$

where χ is the static susceptibility, γ the gyromagnetic ratio, and T the relaxation time. Throughout this paper we make the assumption that the two relaxation times are equal: $T=T_1=T_2$, a condition that is often well satisfied in liquids.[4] As indicated below, the theory is easily extended to the more general case.

In most applications of this theory one will be concerned with a constant magnetic field $\mathbf{H}_0$ in the z direction, with a superimposed alternating field $\mathbf{H}_1$. If the latter oscillates with a single frequency ω, the usual procedure is to transform the problem into an effectively stationary one by passage to a coordinate system rotating about $\mathbf{H}_0$ with angular velocity ω and neglecting the component of $\mathbf{H}_1$ rotating in the opposite direction.[1] Equation (1) remains valid in the rotating system provided we now interpret $\mathbf{H}$ as the "effective" field with components $(H_x, H_y, H_z-\omega/\gamma)$. Our general discussion based on (1) is thus applicable in either the laboratory or the rotating frame.

Equation (1) is cast into matrix form by defining a matrix $\mathfrak{H}(t)$ with the property that $\mathfrak{H}$ operating on any vector has the effect of taking the cross product with $\gamma\mathbf{H}$; symbolically, $\mathfrak{H}=\gamma\mathbf{H}\times$. Thus, in right-handed Cartesian coordinates, $\mathfrak{H}$ takes the form,

$$\mathfrak{H}=\gamma\begin{bmatrix}0 & -H_z & H_y\\ H_z & 0 & -H_x\\ -H_y & H_x & 0\end{bmatrix}. \tag{2}$$

It is often convenient to use the "axial" representation in which a vector M is specified by the components $[M_+=M_x+iM_y, M_-=M_x-iM_y, M_z]$ rather than by the Cartesian $[M_x,M_y,M_z]$. Since the change from one system of representation to another is accomplished by a similarity transformation on all matrices, for example,

$$\mathfrak{H}_{\text{axial}}=\mathbf{S}\mathfrak{H}_{\text{Cartesian}}\mathbf{S}^{-1},$$

with

$$\mathbf{S}=\begin{bmatrix}1 & i & 0\\ 1 & -i & 0\\ 0 & 0 & 1\end{bmatrix},$$

the general relations may be developed without committing ourselves to any particular representation.

The Bloch equations thus appear in matrix form as

$$\frac{\partial \mathbf{M}}{\partial t}+\left[\frac{1}{T}+\mathfrak{H}(t)\right]\mathbf{M}=\mathbf{A}(t), \tag{3}$$

with $\mathbf{A}(t)=\chi\mathbf{H}/T$. If all quantities in (3) were scalars it would reduce to the equation of radioactive decay or of buildup of voltage in an $R-C$ circuit, the general solution of which can be written down immediately; by analogy, we find the solution of the matrix equation. First, we define the time-development matrix $\mathbf{U}(t,t')$,

* Supported in part by the Office of Naval Research.
[1] F. Bloch, Phys. Rev. **70**, 460 (1946): see also Rabi, Ramsey, and Schwinger, Revs. Modern Phys. **26**, 167 (1954).
[2] A. Bloom, following paper [Phys. Rev. **98**, 1104 (1955)].
[3] E. L. Hahn, Phys. Rev. **80**, 580 (1950).
[4] Bloembergen, Purcell, and Pound, Phys. Rev. **70**, 988 (1946).

which satisfies the homogeneous equation,

$$\frac{\partial \mathbf{U}(t,t')}{\partial t}+\left[\frac{1}{T}+\mathfrak{B}(t)\right]\mathbf{U}(t,t')=0, \tag{4}$$

with $\mathbf{U}(t,t)=1$. It is readily verified by substitution that the general solution of (3) is

$$\mathbf{M}(t)=\mathbf{U}(t,0)\mathbf{M}(0)+\int_0^t \mathbf{U}(t,t')\mathbf{A}(t')dt'. \tag{5}$$

To investigate the properties of $\mathbf{U}(t,t')$, note first that the relaxation term may be eliminated from (4) by the transformation,

$$\mathbf{U}(t,t')=\exp[-(t-t')/T]\mathbf{R}(t,t'), \tag{6}$$

and the differential equation satisfied by $\mathbf{R}(t,t')$ is

$$\partial\mathbf{R}(t,t')/\partial t+\mathfrak{B}(t)\mathbf{R}(t,t')=0. \tag{7}$$

According to (7), the value of $\mathbf{R}$ at time $(t+dt)$ is given by

$$\mathbf{R}(t+dt,t')=[1-\mathfrak{B}(t)dt]\mathbf{R}(t,t'),$$

and this process can be repeated indefinitely, leading to the following representation of $\mathbf{R}(t,t')$:

$$\mathbf{R}(t,t')=\lim_{n\to\infty}\left[1-\frac{\tau}{n}\mathfrak{B}\left(t-\frac{\tau}{n}\right)\right]\times\left[1-\frac{\tau}{n}\mathfrak{B}\left(t-\frac{2\tau}{n}\right)\right]\cdots\left[1-\frac{\tau}{n}\mathfrak{B}(t')\right], \tag{8}$$

where $\tau=t-t'$. The matrix $[1-\mathfrak{B}(t)dt]$ represents, according to the definition of $\mathfrak{B}$, an infinitesimal rotation about the instantaneous direction of $\mathbf{H}$ through an angle $\gamma|\mathbf{H}|dt$; therefore, the matrix $\mathbf{R}(t,t')$, being the resultant of an infinite number of such rotations, is a finite rotation matrix, representing the total change of $\mathbf{M}$ that would be produced in the time interval $(t'\to t)$ by Larmor precession if the relaxation and static susceptibility terms were absent.

We note in passing that in consequence of (8), $\mathbf{R}(t,t')$ has the group property

$$\mathbf{R}(t,t')\mathbf{R}(t',t'')=\mathbf{R}(t,t''), \tag{9}$$

and that in the case $\mathfrak{B}(t)=\text{const}$, we have

$$\mathbf{R}(t,t')=\exp[-\mathfrak{B}(t-t')]. \tag{10}$$

The matrix (10), when applied to any vector, carries out a rotation about $\mathbf{H}$ as an axis, through an angle $\gamma|\mathbf{H}|(t-t')$.

III. STEADY SIGNAL

As an illustration of the method, we now evaluate (5) for the case where the magnetic field in the laboratory system is given by $H_x=2H_1\cos\omega t$, $H_y=0$, $H_z=H_0=\text{const}$. This is the situation in which use of the rotating coordinate system is useful; in it the matrix $\mathfrak{B}$ is symbolically $\mathbf{B}\times$, where $\mathbf{B}$ is the vector with components $[\gamma H_1, 0, \gamma H_0-\omega]$. We further assume $H_0\gg H_1$, so that the vector $\mathbf{A}$ in (5) is effectively a constant. The time-development matrix is now, from (6) and (10),

$$\mathbf{U}(t,t')=\lambda(t-t')=\exp\left[-\left(\frac{1}{T}+\mathfrak{B}\right)(t-t')\right], \tag{11}$$

and the integral in (5) is readily evaluated, since the formula for integration of the exponential function applies to matrices as well as to scalars:

$$\int_0^t \lambda(t-t')dt'=[1-\lambda(t)]\left(\frac{1}{T}+\mathfrak{B}\right)^{-1}. \tag{12}$$

Thus, the solution (5) reduces to

$$\mathbf{M}(t)=\lambda(t)[\mathbf{M}(0)-\mathbf{M}(\infty)]+\mathbf{M}(\infty), \tag{13}$$

with the steady-state magnetization given by

$$\mathbf{M}(\infty)=(1/T+\mathfrak{B})^{-1}\mathbf{A}. \tag{14}$$

The inverse of $(1/T+\mathfrak{B})$ may be evaluated by determinants, giving the result,

$$\mathbf{M}(\infty)=\frac{\chi H_0}{1+b^2T^2}\begin{pmatrix} B_xB_zT^2 \\ B_xT \\ 1+B_z^2T^2\end{pmatrix}, \tag{15}$$

where $b\equiv|\mathbf{B}|$. This agrees with the steady-state solution given by Bloch[1] for the case $T_1=T_2$.

To investigate the transient in (13), we note that $\lambda(t)$ represents a rotation about the vector $\mathbf{B}$ through an angle bt, with accompanying exponential decrease in length. Thus, as time goes on, $\lambda(t)\mathbf{A}$ is a vector whose tip describes a spiral on the surface of a cone, as illustrated in Fig. 1. This will be called a λ cone; if the initial polarization is taken as the equilibrium value $\mathbf{M}(0)=\chi\mathbf{H}_0$, it opens out into a disk normal to $\mathbf{B}$. Every transient in the presence of a steady signal is one in which the difference between initial and final polarization decays to zero along a λ cone. The frequency of rotation about the λ cone is

$$b=[(\gamma H_1)^2+(\gamma H_0-\omega)^2]^{\frac{1}{2}},$$

which appears in the laboratory frame as a nutation frequency.

Evidently the general nature of the solution can be understood directly from (13). Finding all details requires explicit evaluation of the matrix $\exp(-\mathfrak{B}t)$. This may be done directly, since its geometrical meaning is already understood, or by making use of the Cayley-Hamilton theorem, according to which each matrix satisfies its own characteristic equation. Since the latter method is general, it is described briefly. If $\mathbf{G}$ is any $(n\times n)$ matrix, its characteristic equation is

$$\det(\mathbf{G}-\lambda 1)=\sum_{k=0}^{n} C_k\lambda^k=0,$$

and therefore

$$\sum_{k=0}^{n} C_k \mathbf{G}^k = 0.$$

By repeated application of this relation any power series in $\mathbf{G}$ may be reduced to a polynomial of degree not exceeding $(n-1)$; thus we know that $\exp(-\beta t)$ is expressible linearly in terms of β, β^2, and the unit matrix:

$$\exp(-\beta t) = a_0(t)\mathbf{1} + a_1(t)\beta + a_2(t)\beta^2. \tag{16}$$

In the present case the characteristic equation of β reduces to

$$\beta^3 + b^2\beta = 0. \tag{17}$$

From (17) and the requirement,

$$\frac{d}{dt}\exp(-\beta t) = -\beta \exp(-\beta t),$$

we find the system of equations $\dot{a}_0 = 0$, $\dot{a}_1 = b^2 a_2 - a_0$, $\dot{a}_2 = -a_1$ with initial conditions $a_0(0) = -\dot{a}_1(0) = 1$, $a_1(0) = a_2(0) = 0$, whose solution gives

$$\exp(-\beta t) = \mathbf{1} - \frac{\sin bt}{b}\beta + \frac{1-\cos bt}{b^2}\beta^2. \tag{18}$$

Thus, multiplication of any vector $\mathbf{A}$ by $\lambda(t)$ results in the vector

$$\lambda(t)\mathbf{A} = e^{-t/T}\left\{\frac{\mathbf{B}(\mathbf{B}\cdot\mathbf{A})}{b^2} + \left[\mathbf{A} - \frac{\mathbf{B}(\mathbf{B}\cdot\mathbf{A})}{b^2}\right]\cos bt - \frac{\mathbf{B}\times\mathbf{A}}{b}\sin bt\right\}. \tag{19}$$

Using this relation, all details of the solution (13) may now be written down. The result, for the y component of magnetization, as seen in the laboratory system, is

$$M_y(t) = \frac{\chi H_0 \omega_1 T}{1+b^2T^2}[\cos\omega t - \Delta\omega T \sin\omega t] + \frac{\chi H_0 \omega_1 T}{b(1+b^2T^2)^{\frac{1}{2}}} \times e^{-t/T}[\Delta\omega \sin(bt+\theta)\sin\omega t - b\cos(bt+\theta)\cos\omega t], \tag{20}$$

where $\omega_1 = \gamma H_1$, $\Delta\omega = \gamma H_0 - \omega$, $\tan\theta = bT$. In the case of resonance ($\Delta\omega = 0$) and strong driving field ($\omega_1 T \gg 1$) the final amplitude is small, but the steady state is well approximated only after many relaxation periods. This problem has previously been treated by Torrey.[5]

It is interesting to note that the form of the general solution (13) corresponds exactly to the solution in simple problems of radioactive decay or buildup of voltage in an $R-C$ circuit. $\lambda(t)$ appears as a matrix analog of the usual exponential damping factor.

[5] H. C. Torrey, Phys. Rev. **76**, 1059 (1949).

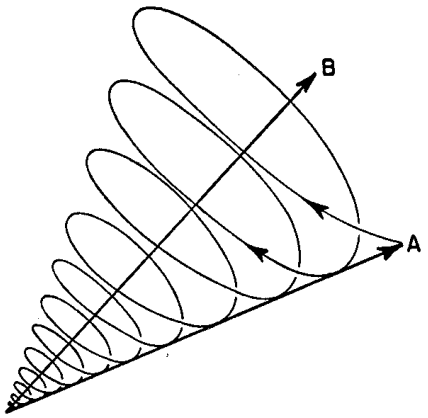

FIG. 1. The λ cone. Locus of the tip of the vector $\lambda(t)\mathbf{A}$ as t varies from 0 to ∞.

IV. GENERAL PERIODIC SIGNAL

To investigate the solution in the case that the magnetic field is an arbitrary periodic function of time, we go back to Eq. (4) and assume β periodic with period τ:

$$\beta(t+\tau) = \beta(t). \tag{21}$$

Then the following relations are consequences of (8)

$$\mathbf{U}(t+n\tau, t'+n\tau) = \mathbf{U}(t,t'), \qquad \mathbf{U}(n\tau,0) = [\mathbf{U}(\tau,0)]^n = \boldsymbol{\alpha}^n(0), \tag{22}$$

where $\boldsymbol{\alpha}(t) = \mathbf{U}(t+\tau, t)$ is the time-development matrix for one period, starting at time t. Writing for brevity, $\mathbf{M}_n(t) = \mathbf{M}(t+n\tau)$, the solution (5) giving the change of M during one period is

$$\mathbf{M}_{n+1}(t) = \mathbf{U}(t+\tau, t)\mathbf{M}_n(t) + \int_{n\tau+t}^{(n+1)\tau+t} \mathbf{U}(t+n\tau+\tau, t')\mathbf{A}(t')dt';$$

or, noting that the integral is independent of n,

$$\mathbf{M}_{n+1}(t) = \boldsymbol{\alpha}(t)\mathbf{M}_n(t) + \mathbf{N}(t), \tag{23}$$

where

$$\mathbf{N}(t) = \int_t^{\tau+t} \mathbf{U}(t+\tau, t')\mathbf{A}(t')dt'. \tag{24}$$

Equation (23) is a simple linear difference equation whose solution is

$$\mathbf{M}_n(t) = \boldsymbol{\alpha}^n[\mathbf{M}_0(t) - \mathbf{M}_\infty(t)] + \mathbf{M}_\infty(t) \tag{25}$$

with the steady-state polarization given by

$$\mathbf{M}_\infty = (1-\boldsymbol{\alpha})^{-1}\mathbf{N}. \tag{26}$$

All eigenvalues of $\boldsymbol{\alpha}$ are less than unity in magnitude, so the term with $\mathbf{M}_0(t)$ in (25) vanishes as $n \to \infty$. Equations (25) and (26) correspond in form to (13) and (14), of which they are a discrete version. Since $\boldsymbol{\alpha}$ is a λ matrix, that is, it represents a combined rotation and exponential shrinking, we see that any transient in the presence of a periodic signal has the following property;

if we look at the polarization only at corresponding instants in each repetition period, we see the difference between initial and final value decaying to zero in discrete jumps along a λ cone. At other times in the repetition period the polarization will not, in general, lie on the same λ cone, but may describe a very complicated path.

The operations represented by α^m and $(1-\alpha)^{-1}$ may be further elucidated by making use of (19). Let the axis of the rotation α be given by the unit vector $\mathbf{n}$, and its magnitude by θ. The matrix α^m applies this rotation m times, so that the result of applying α^m to any vector $\mathbf{A}$ is

$$\alpha^m\mathbf{A}=e^{-mx}\{\mathbf{n}(\mathbf{n}\cdot\mathbf{A})+\sin m\theta(\mathbf{n}\times\mathbf{A}) -\cos m\theta\mathbf{n}\times(\mathbf{n}\times\mathbf{A})\}, \quad (27)$$

where $x\equiv\tau/T$. To get an explicit form for $(1-\alpha)^{-1}$ we use the power series representation,

$$(1-\alpha)^{-1}=\mathbf{1}+\alpha+\alpha^2+\cdots,$$

whose convergence is assured by the exponential damping in α. Thus, the result of applying the operation $(1-\alpha)^{-1}$ to any vector $\mathbf{A}$ is the sum of all the individual vectors in (27). The sums are readily evaluated, with the result

$$\frac{1}{1-\alpha}\mathbf{A}=\frac{\mathbf{n}(\mathbf{n}\cdot\mathbf{A})}{1-e^{-x}}+\frac{\sin\theta}{2(\cosh x-\cos\theta)}(\mathbf{n}\times\mathbf{A}) -\frac{e^x-\cos\theta}{2(\cosh x-\cos\theta)}\mathbf{n}\times(\mathbf{n}\times\mathbf{A}). \quad (28)$$

This expression may be approximated as follows in the case that the repetition period is small compared to the relaxation time ($x\ll 1$). The last two terms of (28) are then small, of the order unity, except when θ is near some multiple of 2π, where they become large, of the order $(1/x)$. When θ is near $2n\pi$, the following approximations are valid:

$$\begin{aligned}\frac{\sin\theta}{2(\cosh x-\cos\theta)}&\simeq\frac{\theta-2n\pi}{x^2+(\theta-2n\pi)^2}=\frac{1}{x}\cos\psi\sin\psi,\\ \frac{e^x-\cos\theta}{2(\cosh x-\cos\theta)}&\simeq\frac{x}{x^2+(\theta-2n\pi)^2}=\frac{1}{x}\cos^2\psi,\end{aligned} \quad (29)$$

where $\tan\psi=(\theta-2n\pi)/x$.

In a coordinate system so oriented that its z axis is parallel to $\mathbf{n}$, $(1-\alpha)^{-1}$ therefore takes the form

$$\frac{1}{1-\alpha}=\frac{1}{x}\begin{bmatrix}\cos^2\psi & -\cos\psi\sin\psi & 0\\ \cos\psi\sin\psi & \cos^2\psi & 0\\ 0 & 0 & 1\end{bmatrix}. \quad (30)$$

Thus, apart from the common factor $1/x$, the operator $(1-\alpha)^{-1}$ does not change the component of $\mathbf{A}$ parallel to $\mathbf{n}$, but the perpendicular components are subjected to a rotation through an angle ψ and decrease in magnitude by a factor of $\cos\psi$. Therefore, we have the following picture of the action of $x(1-\alpha)^{-1}$; when θ is far from $2n\pi$, it merely projects an arbitrary vector $\mathbf{A}$ onto the axis of its λ cone; $x(1-\alpha)^{-1}\mathbf{A}=\mathbf{n}(\mathbf{n}\cdot\mathbf{A})$. When θ approaches a resonance, however, $x(1-\alpha)^{-1}\mathbf{A}$ swings out from $\mathbf{n}$, its tip lying on a circle whose diameter is the projection of $\mathbf{A}$ onto the plane normal to $\mathbf{n}$ (Fig. 2a, 2b). In the usual case, where most of the rotation in one period consists of Larmor precession about the steady field $\mathbf{H}_0$, this resonance phenomenon occurs if the applied signal has a spectral line near the Larmor frequency γH_0.

V. COHERENT PULSES

We now specialize the results of the preceding section to the case where the periodic signal consists of pulses of frequency ω, duration t_1, separated by time intervals t_2 during which only the steady field $\mathbf{H}_0$ is present. It is convenient to regard our relations as pertaining to the rotating coordinate system, as the solution may then be pieced together from solutions of the type (13). Using subscripts 1 and 2 to refer to quantities effective during and between pulses, respectively, two time-development matrices are needed:

$$\lambda_1\equiv e^{-t_1/T}\exp(-\beta_1 t_1), \quad \lambda_2\equiv e^{-t_2/T}\exp(-\beta_2 t_2), \quad (31)$$

with

$$\beta_i=\mathbf{B}_i\times, \quad \mathbf{B}_1=[\gamma H_1, 0, \gamma H_0-\omega], \quad \mathbf{B}_2=[0, 0, \gamma H_0-\omega]. \quad (32)$$

Denoting the polarization at the start and end of the nth pulse by $\mathbf{M}_n$, $\mathbf{M}_n'$, respectively, we then use (13) twice:

$$\mathbf{M}_n'=\lambda_1[\mathbf{M}_n-\mathbf{M}_1(\infty)]+\mathbf{M}_1(\infty),$$
$$\mathbf{M}_{n+1}=\lambda_2[\mathbf{M}_n'-\mathbf{M}_2(\infty)]+\mathbf{M}_2(\infty),$$

in which

$$\begin{aligned}\mathbf{M}_1(\infty)&=(1/T+\beta_1)^{-1}\mathbf{A},\\ \mathbf{M}_2(\infty)&=(1/T+\beta_2)^{-1}\mathbf{A}=\chi\mathbf{H}_0\end{aligned} \quad (33)$$

are, respectively, the steady-state polarizations that would be reached if the signal were left on or off indefinitely. Eliminating $\mathbf{M}_n'$ from these equations, we have the difference equation for $\mathbf{M}_n$; comparing with (23) the result is

$$\begin{aligned}\alpha&=\lambda_2\lambda_1=e^{-\tau/T}\exp(-\beta_2 t_2)\exp(-\beta_1 t_1),\\ \mathbf{N}&=\lambda_2(1-\lambda_1)\mathbf{M}_1(\infty)+(1-\lambda_2)\mathbf{M}_2(\infty).\end{aligned} \quad (34)$$

Therefore, after the transient has died out, we find for the steady-state polarization just at the beginning of the pulse:

$$\mathbf{M}_\infty=\mathbf{M}_1(\infty)+\frac{1}{1-\alpha}(1-\lambda_2)[\mathbf{M}_2(\infty)-\mathbf{M}_1(\infty)]. \quad (35)$$

Evidently an analogous, though more complicated, expression for $\mathbf{M}_\infty$ can be found in this way whenever the applied signal has a constant frequency and a stepwise constant amplitude.

VI. TRANSCRIPTION TO SPINOR REPRESENTATION

Calculation of the resultant of several successive rotations, using the above (3×3) matrices rapidly becomes very tedious. In such evaluation it is a practical necessity to use the two-dimensional representation of the rotation group,[6] also called the Cayley-Klein parameters.[7] To each polarization $\mathbf{M}$, oriented with colatitude and azimuth angles θ, φ, i.e., with components in the axial representation

$$M_+ = M\sin\theta e^{i\varphi},$$
$$M_- = M\sin\theta e^{-i\varphi},$$
$$M_z = M\cos\theta,$$

we associate a spinor[8]

$$\psi = \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} M^{\frac{1}{2}}\cos(\theta/2)e^{-i(\varphi/2)} \\ M^{\frac{1}{2}}\sin(\theta/2)e^{i(\varphi/2)} \end{pmatrix}, \tag{36}$$

and to every rotation of $\mathbf{M}$ generated by a matrix $\mathbf{R}$:

$$\mathbf{M}' = \mathbf{R}\mathbf{M},$$

there corresponds a unitary transformation of ψ:

$$\psi' = \mathbf{Q}\psi.$$

The relation between the elements of $\mathbf{Q}$ and the axis and magnitude of the corresponding rotation is expressed compactly in terms of the Pauli spin matrices,

$$\boldsymbol{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

as follows. The rotation through an angle θ about an axis given by a unit vector $\mathbf{n}$ is represented by the matrix

$$\mathbf{Q} = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix} = \exp[-i(\mathbf{n}\cdot\boldsymbol{\sigma})(\theta/2)]$$
$$= \mathbf{1}\cos(\theta/2) - i(\mathbf{n}\cdot\boldsymbol{\sigma})\sin(\theta/2), \tag{37}$$

or the Cayley-Klein parameters for this rotation are

$$\alpha = \cos(\theta/2) - in_z\sin(\theta/2),$$
$$\beta = -in_-\sin(\theta/2). \tag{38}$$

Alternatively, an arbitrary rotation may be specified by three Eulerian angles; if we carry out in succession a rotation through an angle ξ about the z axis; a rotation η about the x axis, and a rotation ζ about the z axis, the Q-matrix of the resultant is

$$\exp[-i\boldsymbol{\sigma}_z(\zeta/2)]\exp[-i\boldsymbol{\sigma}_x(\eta/2)]\exp[-i\boldsymbol{\sigma}_z(\xi/2)],$$

from which we find

$$\alpha = \cos(\eta/2)\exp[-i(\zeta+\xi)/2],$$
$$\beta = -i\sin(\eta/2)\exp[-i(\zeta-\xi)/2]. \tag{39}$$

The $\mathbf{R}$-matrix corresponding to a given $\mathbf{Q}$-matrix assumes the following form in the axial representation

$$\mathbf{R} = \begin{bmatrix} \delta^2 & -\gamma^2 & 2\gamma\delta \\ -\beta^2 & \alpha^2 & -2\alpha\beta \\ \beta\delta & -\alpha\gamma & (\alpha\delta+\beta\gamma) \end{bmatrix}, \tag{40}$$

where $\delta=\alpha^*$, $\gamma=-\beta^*$.

To aid in evaluating the expressions in the preceding section, we wish to find the Cayley-Klein parameters corresponding to the rotation occurring during a pulse. Referring to Eq. (32), this is a rotation about the vector $\mathbf{B}_1$ through an angle $bt=[(\gamma H_1)^2+(\gamma H_0-\omega)^2]^{\frac{1}{2}}t$. Denoting by φ the angle between the x axis and $\mathbf{B}_1$, Eq. (38) thus reduces to

$$\alpha = \cos(bt/2) - i\sin\varphi\sin(bt/2),$$
$$\beta = i\cos\varphi\sin(bt/2). \tag{41}$$

These relations are used in the following paper for treatment of spin echoes. In terms of the Eulerian angles, we see on comparing (38) and (39) that the condition for the axis of the resultant rotation to lie in the x–z plane is $\xi=\zeta$, so that the Eulerian angles corresponding to the rotation (41) are given by

$$\tan\zeta = \sin\varphi\tan(bt/2),$$
$$\sin(\eta/2) = \cos\varphi\sin(bt/2). \tag{42}$$

Upon using the above results, most of the preceding equations have analogs in the two-dimensional representation scheme. The correspondence is determined by that for infinitesimal rotations: if $\beta=\mathbf{B}\times$, we have from (37)

$$[1-\beta dt] \rightarrow [1-\tfrac{1}{2}i(\boldsymbol{\sigma}\cdot\mathbf{B})dt],$$

and therefore a finite rotation matrix is given by

$$\mathbf{Q}(t,t') = \lim_{\tau\rightarrow 0}[1-\tfrac{1}{2}i\tau\boldsymbol{\sigma}\cdot\mathbf{B}(t-\tau)]$$
$$\times[1-\tfrac{1}{2}i\tau\boldsymbol{\sigma}\cdot\mathbf{B}(t-2\tau)]\cdots[1-\tfrac{1}{2}i\tau\boldsymbol{\sigma}\cdot\mathbf{B}(t')]. \tag{43}$$

It satisfies the differential equation

$$\partial Q(t,t')/\partial t + \tfrac{1}{2}i\boldsymbol{\sigma}\cdot\mathbf{B}(t)\mathbf{Q}(t,t') = 0, \tag{44}$$

which may also be derived from the fact that in the limit of infinite relaxation time, the spinor (36) satisfies the Schrödinger equation for a particle of spin $\frac{1}{2}$.

[6] E. P. Wigner, *Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren* (Friedrick Vieweg, & Sohn, Braunschweig, 1931), Chap. XV.

[7] H. Goldstein, *Classical Mechanics* (Addison-Wesley Press, New York, 1951).

[8] H. A. Kramers, *Quantentheorie des Elektrons und der Strahlung* (Akademische Verlagsgesellschaft, Leipzig, 1938), Chap. 6.

Since the matrix

$$\tfrac{1}{2}i\boldsymbol{\sigma}\cdot\mathbf{B}=\tfrac{1}{2}i\begin{pmatrix}B_z & B_- \\ B_+ & -B_z\end{pmatrix} \tag{45}$$

corresponds to the 3×3 matrix $\mathfrak{B}$ in all the above relations, it will also be denoted as $\mathfrak{B}$ in what follows; it will be clear from the context whether we are using the two- or three-dimensional representation. Thus, for example, the rotation matrix (37) may be written as $\exp(-\mathfrak{B}t)$, where $\mathbf{n}\theta=\mathbf{B}t$.

VII. APPROXIMATE SOLUTIONS

In most problems that arise we have a strong constant field $\mathbf{H}_0$, whose direction we choose as the z-axis, plus a weak varying field $\mathbf{H}_1(t)$. Therefore in (7) we write $\mathfrak{B}(t)=\mathfrak{B}_0+\mathfrak{B}_1(t)$, and the major part of the time variation of $\mathbf{R}(t,t')$ or $\mathbf{Q}(t,t')$ is a uniform Larmor precession due to $\mathfrak{B}_0$. When we use the two-dimensional representation, this can be removed from the equation of motion (44) by the transformation

$$\mathbf{Q}(t,t')=\exp[-\mathfrak{B}_0t]\mathbf{Q}'(t,t')\exp[+\mathfrak{B}_0t'], \tag{46}$$

whereupon $\mathbf{Q}'$ satisfies the relation

$$\partial\mathbf{Q}'(t,t')/\partial t+\mathfrak{B}'(t)\mathbf{Q}'(t,t')=0, \tag{47}$$

with

$$\mathfrak{B}'(t)=\exp[\mathfrak{B}_0t]\mathfrak{B}_1(t)\exp[-\mathfrak{B}_0t], \tag{48}$$

and $\mathbf{Q}'(t,t)=1$. This is analogous to passage to the rotating coordinate system discussed in Sec. II, but differs from it in several respects; for example, the rotation frequency is here always $\omega_0=\gamma H_0$ rather than the applied frequency. Since $\mathbf{Q}'$ is only slowly varying if $H_1\ll H_0$, an approximate solution of (47) using a finite number of terms of the expansion

$$\mathbf{Q}'(t,t')=\mathbf{1}-\int_{t'}^{t}dt''\mathfrak{B}'(t'')+\int_{t'}^{t}dt''\mathfrak{B}'(t'')\times\int_{t'}^{t''}dt'''\mathfrak{B}'(t''')+\cdots \tag{49}$$

is valid for a much longer time interval than is the corresponding approximate solution of (44). Equation (49) is now used to evaluate $\mathbf{Q}$ for the case that the variable field $\mathbf{H}_1(t)$ lies in the x–y plane. Then, writing $\omega_0=\gamma H_0$, we find $\mathfrak{B}(t)=\mathbf{B}\times$, where $B_\pm(t)=\gamma H_\pm(t)\times\exp(\pm i\omega_0t)$, $B_z=0$. When we write out (49), the Cayley-Klein parameters for $\mathbf{Q}'$ are

$$\alpha'=1-\tfrac{1}{4}\gamma^2\int_{t'}^{t}dt''\int_{t'}^{t''}dt'''H_-(t'')H_+(t''')\times\exp[i\omega_0(t'''-t'')], \tag{50}$$

$$\beta'=-\tfrac{1}{2}i\gamma\int_{t'}^{t}dt''H_-(t'')\exp(-i\omega_0t''), \tag{51}$$

in which all terms through the second order of $\mathfrak{B}'$ are retained. From (46), the parameters of $\mathbf{Q}(t,t')$ are

$$\alpha=\alpha'\exp[-i\omega_0(t-t')/2], \tag{52}$$

$$\beta=\beta'\exp[-i\omega_0(t+t')/2]. \tag{53}$$

As shown in the following paper, it is the product of (52) and (53) that is needed for interpretation of experiments in which one observes the effect of a signal which has been impressed for a time short compared to the relaxation time.

For time intervals containing many Larmor periods, the integrals in (50), (51) are well approximated in terms of the Fourier transforms of $H_-(t)$. To fix reasonable orders of magnitude of these terms, we consider the case of protons in water, in a magnetic field such that the Larmor frequency is about 30 megacycles/sec, while a weak signal $H_-(t)$ is applied with a repetition rate of about 1000 sec^{-1}, the relaxation time being of the order of a second. Then we are interested in evaluating (50), (51) for time intervals t_1 for which

$$\begin{aligned}\omega_0t_1&\sim10^4,\\ \gamma H_-t_1&\sim1,\end{aligned} \tag{54}$$

and there is a wide range of conditions under which the relations $t_1/T\ll\gamma H_-t_1\ll\omega_0t_1$ are valid. If $H_-(t)$ is represented by a Fourier integral,

$$H_-(t)=\int_{-\infty}^{\infty}G(\omega)\exp(i\omega t)d\omega, \tag{55}$$

we may substitute into (50), (51) and perform the time integrations. Approximations of the form

$$\lim_{t\to\infty}\frac{\exp(i\omega t)-1}{i\omega}=\pi\delta(\omega)$$

will be valid, leading to the simplified expressions:

$$\alpha'=1-\tfrac{1}{8}\pi^2\gamma^2(t-t')^2|G(\omega_0)|^2, \tag{56}$$

$$\beta'=-\tfrac{1}{2}i\pi\gamma(t-t')G(\omega_0). \tag{57}$$

Suppose that after a certain time interval the applied field $H_-(t)$ is turned off. Thereafter, in (52) and (53), α' and β' remain constant at the values fixed by (56), (57), and so the product $\alpha\beta$ continues to oscillate at frequency ω_0 with amplitude $\alpha'\beta'$. If this amplitude contains terms whose phase varies linearly with ω_0, then in an inhomogeneous field where nuclei with all values

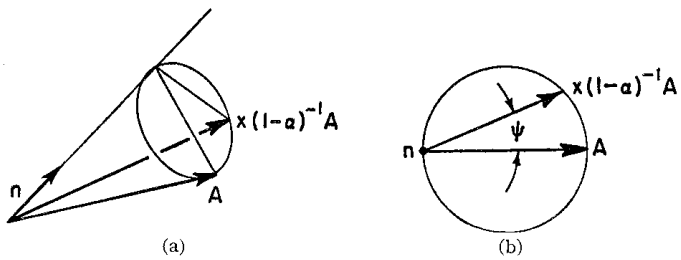

FIG. 2. (a) Circle traversed by $(\mathbf{1}-\boldsymbol{\alpha})^{-1}\mathbf{A}$ as θ sweeps through each resonance. (b) Projection of (a) on a plane normal to $\mathbf{n}$.

of ω_0 are present, one finds "coherences," or "echoes" as described in the following paper.

VIII. GENERALIZATION FOR $T_1 \neq T_2$

The assumption that the two relaxation times are equal has simplified our geometric interpretations, but the analytical expressions in the 3×3 representation remain almost as simple if it is dropped. Thus, the equation of motion (3) remains valid provided we interpret $1/T$ as a diagonal matrix with elements $[1/T_2,1/T_2,1/T_1]$. Equations (4), (5), (16) then remain valid although $\mathbf{R}(t,t')$ is no longer a pure rotation matrix. The time-development matrix $\mathbf{U}(t,t')$ is given by an expression of the form (8) in which $\mathfrak{z}$ is replaced by $(\mathbf{T}^{-1}+\mathfrak{z})$, and the solution (13) is valid, with $\mathfrak{a}(t) = \exp[-(\mathbf{T}^{-1}+\mathfrak{z})t]$. The locus generated by $\mathfrak{a}(t)$ is now a distorted version of a cone. Similarly, the relations (22)–(26) of Sec. IV still hold, although the geometrical picture is less simple.