Shapes of Nuclear Induction Signals*

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The various shapes of nuclear induction signals are discussed for small values of the r-f field. In the case of a linear variation with time of the strong magnetic field, numerical results are given for various values of the sweep rate and the total relaxation time.

1. INTRODUCTION

THE equations of motion of the total nuclear magnetic moment in the nuclear induction experiment have been given by Bloch.[1] He discusses the solution for the adiabatic case, i.e., when the rate of change of the strong magnetic field is sufficiently small. However, for rapid variations of the strong field, oscillations are experimentally observed in the tails of the curves. These were first explained by Purcell,[2] who pointed out that when the magnetic moment does not have time to follow the adiabatic solution through resonance, the moment will be found pointing in a non-equilibrium direction when the strong field is so far beyond resonance that the effect of the rotating field can be neglected. From this point on the moment will precess about the direction of the strong field, with a damping determined by the relaxation time and with the instantaneous Larmor frequency. The beats between this varying frequency and that of the r-f field will appear as damped oscillations on an oscilloscope screen. In the course of our detailed discussion of these oscillations it will be shown that in certain cases they can be used for a relatively accurate determination of the total relaxation time.

We shall consider the case where the r-f field is weak enough to be treated as a small perturbation. The equations can then be solved for arbitrary dependence of the sweep field on the time. The use of a weak r-f field can be of advantage, since it enables one to obtain the sharpest possible lines. A detailed analysis of the signal shape for this case is of considerable importance since, as long as there remain essential features in the line shape which are unexplained,[3] a resonance value can hardly be known with a limit of error less than the line width.

2. SYMMETRY PROPERTIES OF THE EQUATIONS

The equations of motion of the magnetic moment of a collection of nuclei in a homogeneous magnetic field $H_0(t)$ in the z direction, acted upon by a rotating magnetic field of amplitude H_1 and angular frequency ω, are:[1]

$$(du/dt)+(u/T_2)+(\Delta\omega)v=0, \qquad (1a)$$

$$(dv/dt)+(v/T_2)-(\Delta\omega)u=-|\gamma|H_1M_z, \qquad (1b)$$

$$(dM_z/dt)+(M_z/T_1)-|\gamma|H_1v=M_0/T_1. \qquad (1c)$$

u and v are components of the magnetic moment in- and out-of-phase, respectively, with the rotating field H_1; $|\gamma|$ is the absolute value of the gyromagnetic ratio; $\Delta\omega=|\gamma|H_0(t)-\omega$; and $M_0=\chi H_0$ is the equilibrium polarization. In practice, the percentage variation in H_0 is very small, and M_0 will be treated as a constant. Finally, T_1 is the longitudinal relaxation time which governs the approach to thermal equilibrium, and T_2 is the "transverse relaxation time" which contributes only to the broadening of the resonance line.

Equations (1) possess a symmetry property of considerable practical interest. Suppose that $\Delta\omega(t)$ is a periodic function of the time with period τ, and further that $\Delta\omega(t+\tau/2)=-\Delta\omega(t)$ for all times t. Then, if $u(t)$, $v(t)$ and $M_z(t)$ are a solution of Eqs. (1), the functions $-u(t+\tau/2)$, $v(t+\tau/2)$, and $M_z(t+\tau/2)$ are likewise solutions. This can be seen from direct substitution into the equations provided that the very small variation in M_0 is neglected. The most general

* Work supported by grants from the Office of Naval Research.
[1] F. Bloch, Phys. Rev. 70, 460 (1946).
[2] To be published soon; previous verbal communication to Professor Bloch.
[3] A. Roberts, Phys. Rev. 72, 979 (1947).

solutions of (1) consist of a superposition of a damped homogeneous solution and an inhomogeneous solution. It will be only the latter which is left after initial transients have damped out and it must, therefore, possess the above property of even periodicity in a half-cycle $\tau/2$ for v and M_z, and "odd" periodicity for u. Seen on the screen of an oscilloscope, the horizontal sweep of which has the same periodicity as $\Delta\omega$, the v traces will thus appear symmetrical about the resonance point at the center of the screen while the u trace will be antisymmetrical, once stationary conditions have established themselves. Either phase can, of course, be observed by proper phase adjustment in the receiver circuit.

This property, since it is independent of the magnitudes of H_1, T_1, T_2 or the rate of sweep, is quite useful in practice. For example, one may wish to compare the resonance frequencies of two different nuclei simultaneously in the same magnetic field.[4] It is not always practicable to adjust the parameters so that simple line shapes are seen. A sinusoidal sweep, however, has the property that $\Delta\omega(t+\tau/2)=-\Delta\omega(t)$, provided that one sweeps equally on either side of resonance. If one, therefore, uses the v mode and adjusts the r-f frequencies so that the two sets of traces are completely symmetrical about a common symmetry point, one has a very sensitive method of ascertaining that the two resonances occur at the same value of H_0. In this way, the proton-deuteron magnetic moment ratio has been determined[5,6] with a precision much better than that given by the line widths.

3. SOLUTION OF THE EQUATIONS

Equations (1a) and (1b) can be rewritten in terms of a complex function $F=v+iu$ as follows:

$$(dF/dt)+[(1/T_2)+i\Delta\omega(t)]F=-|\gamma|H_1M_z, \quad (2)$$

which has the solution

$$F=-|\gamma|H_1\int_{-\infty}^{t}dt'M_z(t')\times\exp\left[-(t-t'/T_2)-i\int_{t'}^{t}\Delta\omega(t'')dt''\right]. \quad (3)$$

[4] F. Bloch, A. C. Graves, M. Packard, and R. W. Spence, Phys. Rev. **71**, 551 (1947).
[5] F. Bloch, E. C. Levinthal, and M. E. Packard, Phys. Rev. **72**, 1125 (1947).
[6] F. Bitter, Alpert, Nagle, and Poss, Phys. Rev. **72**, 1271 (1947).

In our case, H_1 is small enough so that the effect of the rotating field can be treated as a small perturbation. We see from (3) and (1c) that, to terms proportional to $(H_1)^2$, one can take for M_z the approximately constant value M_0, so that in this approximation

$$v+iu=-|\gamma|H_1M_0\int_{-\infty}^{t}dt'\times\exp\left[-(t-t'/T_2)-i\int_{t'}^{t}\Delta\omega(t'')dt''\right]. \quad (4)$$

Experimental conditions for which this approximate solution is valid can be obtained by decreasing the r-f power until the shape of the signal remains unchanged and its magnitude varies proportional to H_1.

It is interesting to see that the solution (4) can be found from a slightly different viewpoint. Following Bloch,[1] one can think of the transverse relaxation time effects as due to an effective inhomogeneity in H_z. If $N(H')dH'$ is the fraction of nuclei for which H_z lies between $H_0(t)+H'$ and $H_0(t)+H'+dH'$, and also, if $u(t,H')dH'$, for example, is the in-phase component of the total moment of such nuclei, then Eqs. (1) can be replaced by

$$\frac{du(H')}{dt}+\frac{u(H')}{T_1}+(\Delta\omega+|\gamma|H')v(H')=0, \quad (5a)$$

$$\frac{dv(H')}{dt}+\frac{v(H')}{T_1}-(\Delta\omega+|\gamma|H')u(H')=-|\gamma|H_1M_z(H'), \quad (5b)$$

$$\frac{dM_z(H')}{dt}+\frac{M_z(H')}{T_1}-|\gamma|H_1v(H')=(M_0/T_1)N(H'). \quad (5c)$$

Rewriting (5a) and (5b) in a form corresponding to (3), we find for the total v and u

$$v+iu=\int_{H'}[v(H')+iu(H')]dH'=-|\gamma|H_1\int_{-\infty}^{t}dt'\exp\left[-\frac{t-t'}{T_1}-i\int_{t'}^{t}\Delta\omega(t'')dt''\right]\int_{H'}M_z(t',H')\times\exp[-i(t-t')|\gamma|H']dH'.$$

For strong r-f fields the above expression is not equivalent to (3) for any plausible choice of $N(H')$, and Eqs. (1) are not, in general, mathematically equivalent to an effective inhomogeneity in H_z. However, for very small H_1 we have $M_z(H')\cong M_0N(H')$. If one assumes a broadening of the simple form

$$N(H')dH'=1/\pi[\Gamma dH'/(H')^2+\Gamma^2],$$

one again obtains Eq. (4) with neglect of terms proportional to $(H_1)^3$; T_2 is now given by $1/T_2=(1/T_1)+|\gamma|\Gamma$.

4. ASYMPTOTIC BEHAVIOR

The general characteristics of the solution far from resonance can be seen immediately by performing an integration by parts on (4) which yields

$$v+iu=-\frac{|\gamma|H_1T_2M_0(1-i\Delta\omega T_2)}{1+(\Delta\omega T_2)^2}-i|\gamma|H_1M_0\times\exp\left[-\frac{t}{T_2}-i\int_b^t\Delta\omega''dt''\right]\int_{-\infty}^t dt'\exp\left[\frac{t'}{T_2}+i\int_b^{t'}\Delta\omega''dt''\right]\frac{d\Delta\omega'/dt'}{[(1/T_2)+i\Delta\omega']^2}. \quad (6)$$

If two times τ_1 and τ_2 exist, so that

$$\frac{d\Delta\omega'/dt'}{(1/T_2)^2+(\Delta\omega')^2}\ll 1 \quad (7)$$

for $\tau_1<t'<\tau_2$, then the integral in (6) is roughly constant for times t between τ_1 and τ_2, and

$$v(t)+iu(t)\approx-\frac{|\gamma|H_1T_2M_0(1-i\Delta\omega T_2)}{1+(\Delta\omega T_2)^2}-B\exp\left[-\frac{t}{T_2}-i\int_b^t\Delta\omega''dt''\right],\quad \tau_1<t<\tau_2; \quad (8)$$

$$B=i|\gamma|H_1M_0\int_{-\infty}^{\tau_1}dt'\times\exp\left[\frac{t'}{T_2}+i\int_b^{t'}\Delta\omega''dt''\right]\frac{d\Delta\omega'/dt'}{[(1/T_2)+i\Delta\omega']^2}.$$

The first term of this solution represents the familiar contribution obtained from slow passage, and is seen to depend only on the instantaneous value of $\Delta\omega(t)$. Upon this contribution is superimposed a damped free oscillation which is excited by the passage through resonance. The amplitude and phase of this oscillation will of course depend on the explicit time dependence of $\Delta\omega$. In the case that T_2 is shorter than about $\frac{1}{4}$ cycle of the sweep, the oscillations will have been damped out before $\Delta\omega(t)$ becomes so small that (7) is no longer valid, and the signals will be seen to have oscillations immediately after resonance and none before resonance. The occurrence of the damping factor in (8) provides a method for measuring T_2 in favorable cases.

In the limiting case where $(d\Delta\omega/dt)(T_2)^2$ is at all times negligible one has the situation of slow passage without the excitation of transient oscillations.

5. LINEAR SWEEP

In practice, the strong magnetic field may be swept sinusoidally back and forth about resonance. If the total relaxation time T_2 is less than about one-tenth of the sweep period, the periodicity and the variation of $d\Delta\omega/dt$ can be neglected, and the sweep can be approximated by a linear function of the time.

We shall let $\Delta\omega=at$ where

$$a=|\gamma|(dH_0/dt)_{\text{resonance}}$$

and consider only positive values of a; for a negative, the only change is in the sign of u. If we introduce the dimensionless quantities

$$x=a^{\frac{1}{2}}t,\quad A=1/(a^{\frac{1}{2}}T_2), \quad (9)$$

and express all components of the magnetic moment in units of M_0, (4) becomes

$$v+iu=-(|\gamma|H_1/a^{\frac{1}{2}})\exp[-Ax-i(x^2/2)]\times\int_{-\infty}^{x}\exp[Ax'+i(x'^2/2)]dx'$$
$$=-(|\gamma|H_1/a^{\frac{1}{2}})2^{\frac{1}{2}}\exp[-i\pi/4-z_0^2]\times\int_{(\infty)\exp[-3\pi i/4]}^{z_0}\exp[z^2]dz; \quad (10)$$

$$z_0=(1/2^{\frac{1}{2}})(xe^{i\pi/4}+Ae^{-i\pi/4}). \quad (11)$$

Thus, the solution is expressed in terms of the error function of complex argument.

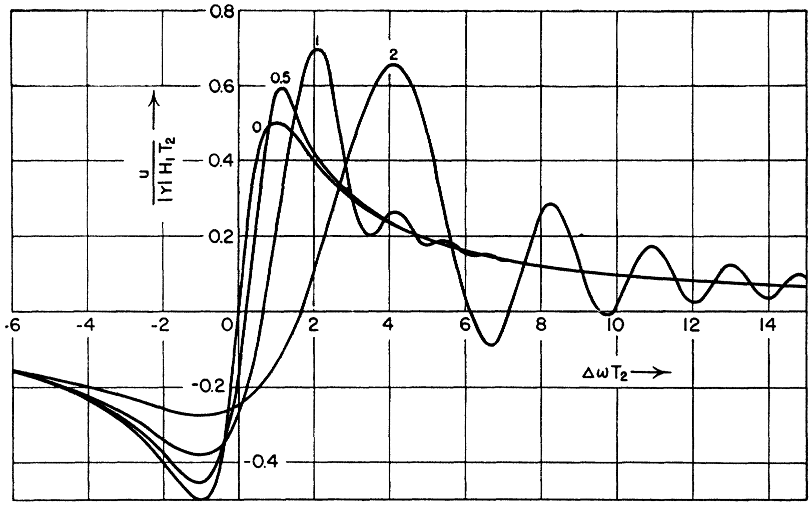

FIG. 1. In-phase resonance shapes (small r-f field and linear sweep) for various values of $a^{\frac{1}{2}}T_2$ given by the numbers near the first maximum. u = in-phase component; T_2 = total relaxation time; $\Delta\omega = at$ = deviation from resonance angular frequency; H_1 = amplitude of rotating r-f field; and $|\gamma|$ = absolute value of gyromagnetic ratio.

For $A=0(T_2=\infty)$, v and u can be expressed in terms of the Fresnel integrals.[7] Values at the points $x=\pm A$ and 0 can likewise be expressed in terms of tabulated functions:

$$u(-A)=v(-A)=-(|\gamma|H_1/a^{\frac{1}{2}})(\pi^{\frac{1}{2}}/2)\times[\exp A^2][1-\operatorname{erf}(A)];\quad (du/dx)_{-A}=0. \tag{12}$$

$$\left.\begin{matrix}u(0)\\ v(0)\end{matrix}\right\}=-(|\gamma|H_1/a^{\frac{1}{2}})\times\pi^{\frac{1}{2}}\left[\left\{\begin{matrix}\cos(A^2/2)\\ -\sin(A^2/2)\end{matrix}\right\}(\tfrac{1}{2}-C(A^2/2))+\left\{\begin{matrix}\sin(A^2/2)\\ \cos(A^2/2)\end{matrix}\right\}(\tfrac{1}{2}-S(A^2/2))\right]. \tag{13}$$

$$\left.\begin{matrix}u(A)\\ v(A)\end{matrix}\right\}=-(|\gamma|H_1/a^{\frac{1}{2}})\times[\exp-A^2]\left[(\pi^{\frac{1}{2}}/2)\mp\int_0^A \exp z^2dz\right]. \tag{14}$$

C and S are the Fresnel integrals.[8]

By performing successive integrations by parts on (10), one finds the following asymptotic expressions, valid when $A^2+x^2\gg 1$:

$$u=\left\{\begin{matrix}1\\0\end{matrix}\right\}\frac{|\gamma|H_1}{a^{\frac{1}{2}}}(2\pi)^{\frac{1}{2}}\exp[-t/T_2]\times\sin\left(\frac{x^2-A^2}{2}-\frac{\pi}{4}\right)+\frac{|\gamma|H_1T_2(\Delta\omega T_2)}{1+(\Delta\omega T_2)^2}+\frac{|\gamma|H_1}{a^{\frac{1}{2}}}\left\{\frac{\sin 3\theta}{(A^2+x^2)^{\frac{3}{2}}}-\cdots\right\},$$

$$v=\left\{\begin{matrix}1\\0\end{matrix}\right\}\frac{|\gamma|H_1}{a^{\frac{1}{2}}}(2\pi)^{\frac{1}{2}}\exp[-t/T_2]\times\cos\left(\frac{x^2-A^2}{2}-\frac{\pi}{4}\right)-\frac{|\gamma|H_1T_2}{1+(\Delta\omega T_2)^2}+\frac{|\gamma|H_1}{a^{\frac{1}{2}}}\left\{\frac{\cos 3\theta}{(A^2+x^2)^{\frac{3}{2}}}+\cdots\right\}, \tag{15}$$

$$0\leqslant\theta=\arctan(A/x)\leqslant\pi.$$

TABLE I. In-phase component u.

	First maximum		First minimum	
$a^{\frac{1}{2}}T_2$	$x=\Delta\omega/a^{\frac{1}{2}}$	$(a^{\frac{1}{2}}/\|\gamma\|H_1)u$	x	$(a^{\frac{1}{2}}/\|\gamma\|H_1)u$
0.5	2.32	0.296	...	...
1.0	2.06	0.697	3.45	0.202
2.0	2.08	1.303	3.35	−0.178
∞	2.14	2.93	3.32	−2.22

TABLE II. Out-of-phase component v.

	First maximum		First minimum	
$a^{\frac{1}{2}}T_2$	$x=\Delta\omega/a^{\frac{1}{2}}$	$-(a^{\frac{1}{2}}/\|\gamma\|H_1)v$	x	$-(a^{\frac{1}{2}}/\|\gamma\|H_1)v$
0.5	0.60	0.49	...	...
1.0	1.00	0.866	2.92	−0.058
2.0	1.09	1.323	2.78	−0.590
∞	1.32	2.33	2.80	−2.54

[7] F. Bitter *et al.*, M.I.T. Research Laboratory of Electronics, Quarterly Progress Report, July 15, 1947, p. 26.

[8] Jahnke and Emde, *Tables of Functions* (Dover Publications, New York, 1945), pp. 35–36.

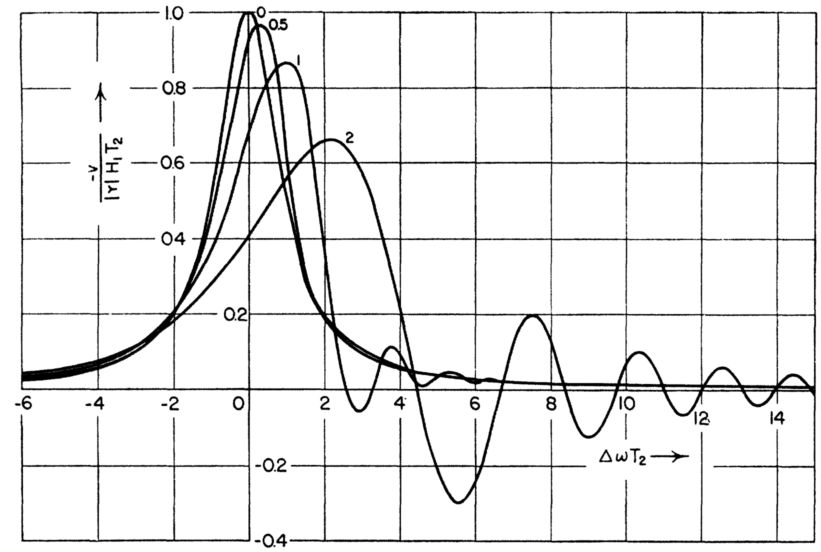

FIG. 2. Out-of-phase resonance shapes (small r-f field and linear sweep) for various values of $a^{\frac{1}{2}}T_2$ given by the numbers near the first maximum. v = out-of-phase component. Other symbols same as for Fig. 1.

The coefficient of the damped oscillation is 1 for $x>A$, while the term is absent for $x<A$. At $x=A$, the discontinuity in Eq. (15) is of the same order as the error in the semiconvergent sums.

Equations (12) through (15) are sufficient to cover most of the range of values of x, except for the first maximum and minimum beyond resonance. In these cases, the integrals (10) were found by following an integration path through the origin and making an angle of $+45°$ with the real axis (Fresnel integrals), and then from an appropriate point integrating numerically along a $-45°$ angle path to the point z_0.

6. RESULTS

The curves for u and $-v$ for various values of $a^{\frac{1}{2}}T_2$ are shown in Figs. 1 and 2, plotted against $\Delta\omega T_2 = x/A$. The free oscillations are completely damped out for $a^{\frac{1}{2}}T_2 \leqslant \frac{1}{2}$.

For $a^{\frac{1}{2}}T_2 \sim 1$, the ratio of the first maximum of u and $-v$ to the first minimum serves as a fairly sensitive measurement of the total relaxation time. These values are given in Tables I and II.

For values of $a^{\frac{1}{2}}T_2 \geqslant \sim 2$, the free oscillations about the slow passage tail appear far enough out so that the total relaxation time can be measured from their damping rate.

The curves shown in Figs. 1 and 2 were in existence when measurements on the proton-deuteron magnetic moment ratio were made at Stanford.[5] It was realized that, because of their smaller gyromagnetic ratio, the relaxation time due to the presence of paramagnetic ions had to be appreciably longer for the deuterons than for the protons in the same sample. The agreement between the aspect of the theoretical curves and that of the signals which were observed lent confidence to the precision attached to the experimental results.

We wish to thank Professor F. Bloch for suggesting this problem and for many valuable discussions concerning it.