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Study of NMR Line Shapes by Using Equivalent Circuit Model Approach*

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Abstract: NMR is a very powerful tool for the study of local dynamics. The nuclear magnetic susceptibility $(\chi = \chi' - j\chi'')$ of a material having spin system obeying Bloch equations is given by [1, 2]

(1) $\chi' = (1/2)\chi_0\omega_0 T_2 \left[(\omega_0 - \omega) T_2 \Big/ \left(1 + (\omega - \omega_0)^2 T_2^2\right)\right]$,

(2) $\chi'' = (1/2)\chi_0\omega_0 T_2 \left[1 \Big/ \left(1 + (\omega - \omega_0)^2 T_2^2\right)\right]$,

where, χ_0 , ω_0 , ω and T_2 are ,respectively , the static magnetic susceptibility of the spin system, Larmor frequency , angular frequency of the externally applied radio frequency field and spin- spin relaxation time. The inductance of a coil filled with such a material is given by

(3) $L = L_0 \left(1 + 4\pi\chi(\omega)\right)$,

where L_0 is inductance of empty coil.
Denoting the coil resistance in the absence of a sample as R_0, the coil impedance $Z^* = Z' - jZ''$ becomes

(4) $Z^* = R_0 + 4\pi L_0 \omega\chi'' + jL_0\omega(1 + 4\pi\chi')$.

The real and imaginary parts of the NMR signal would be proportional to χ'' and χ' .It can be shown from equation (1) and (2) that χ' and χ'' satisfies the following equation

(5) $(\chi'' - \chi_0\omega_0 T_2/4)^2 + (\chi')^2 = (\chi_0\omega_0 T_2/4)^2$,

which is equation of a circle with center at ($\chi_0\omega_0 T_2$ /4,0) and radius $\chi_0\omega_0 T_2$ /4 in the χ' vs. χ'' plot. Any deviation of the experimental plot from circular shape indicate that more than one spin-spin relaxation times are present in the system or

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Bloch equations are not obeyed by the spin system. It is shown that such a plot can be simulated by using combinations of LCR elements. It is proposed that the NMR lines for which circular arcs are not obtained may be studied by using higher resolution spectrometers or by analyzing the data by using equivalent circuit models.
Keywords: NMR Line Shapes, DISPA Plot, Spin-Spin Relaxation Time, Bloch Equations, Equivalent Circuit Model.

1. Introduction

Bloch equations[3] describing NMR phenomenon are

(6)
$$dM_z/dt = -\gamma M_y H_1 + (M_0 - M_z)/T_2$$
$$dM_x/dt = \gamma M_y h_0 - M_x/T_2$$
$$dM_y/dt = \gamma(M_z H_1 - M_z h_0) - M_y/T_2$$

where the terms have usual meaning and $h_0 = H_0 + (\omega_z/\gamma)$.
Writing $M_0 = \chi_0 H_0$, $\omega_0 = \gamma H_0$, $\omega_z = -\omega$, we get for steady state

$$M_x = \chi_0 \omega_0 T_2 \left[(\omega_0 - \omega)T_2 / \left(1 + (\omega - \omega_0)^2 T_2^2\right)\right] H_1,$$
(7)
$$My = \chi_0 \omega_0 T_2 \left[1/\left(1 + (\omega - \omega_0)^2 T_2^2\right)\right] H_1,$$

Remembering that laboratory component M_X is related to the components M_x and M_y in the rotating frame as

(8) $$M_x = M_x \cos \omega t + M_y \sin \omega t.$$

The fields are given as

(9) $$H_x(t) = H_{x0} \cos \omega t, 2H_1 = H_{x0}$$

and writing

(10) $$M_x(t) = (\chi' \cos \omega t + \chi'' \sin \omega t).$$

We get the susceptibilities as given by Eq. (1) and (2).
Similar expressions are obtained for displacement in the case of driven damped harmonic oscillator.

Equation of motion of a damped harmonic oscillator of mass m, spring constant k, damping coefficient f and being driven by a force $F_0 \cos \omega t$ is given by

(11) $$md^2x/dt^2 + f\,dx/dt + kx = F_0 \cos \omega t.$$

The steady state solution is of the form

(12) $$x = x' \cos \omega t + x'' \sin \omega t,$$

where

(13) $$x' = F_0 \left[m\left(\omega_0^{\,2} - \omega^2\right) / \, m^2\left(\omega_0^{\,2} - \omega^2\right)^2 + f^2\omega^2 \right],$$

(14) $$x'' = F_0 \left[f\omega \,/ \left(\left(\omega_0^{\,2} - \omega^2\right)^2 + f^2\omega^2\right)\right].$$

When the frequency ω of the driving force is close to the resonance frequency ie $\omega \sim \omega_0$ and $|\omega_0 - \omega| << |\omega_0 + \omega|$, these expressions reduce to

(15) $$x' = \left(F_0 / \left(2 m \omega_0\right)\right)\left[\left(\omega_0 - \omega\right)\tau \,/ \left(1 + \left(\omega_0 - \omega\right)^2 \tau^2\right)\right],$$

(16) $$x'' = \left(F_0 / \left(2 m \omega_0\right)\right)\left[\tau \,/ \left(1 + \left(\omega_0 - \omega\right)^2 \tau^2\right)\right].$$

If we replace “m”, “f ”, and “k” by “L”, “ R” and “$1/C$ ” respectively, displacement “ x” by charge “q” and $F_0 \cos \omega t$ by $V_0 \cos \omega t$, Eq. (11\`) represents a driven LCR network. The steady state values of charge “ q” is given by

(17) $$q(t) = \left(V_0 / \left(2 L \omega_0\right)\right)\left[\left\{\left(\omega_0 - \omega\right)\tau \,/ \left(1 + \left(\omega_0 - \omega\right)^2 \tau^2\right)\right\}\cos \omega t\right] + \left\{\tau \,/ \left(1 + \left(\omega_0 - \omega\right)^2 \tau^2\right)\right\}\cos \omega t$$

Magnitudes of in-phase and out of phase currents would be [4, 5]

In phase

(18) $$\left(V_0 / 2L\right)\left\{\tau \,/ \left(1 + \left(\omega_0 - \omega\right)^2 \tau^2\right)\right\}$$

Out of phase

(19) $$\left(V_0 / 2L\right)\left\{\left(\omega_0 - \omega\right)\tau \,/ \left(1 + \left(\omega_0 - \omega\right)^2 \tau^2\right)\right\}$$

These are similar to the expressions for χ’’ and χ’ respectively given in Eq. (1) and (2).Thus NMR phenomenon can be modeled by an equivalent circuit where the driving force $F_0 \cos \omega t$ or $V_0 \cos \omega t$ would be proportional to the H_1 field produces by the NMR coil.

The receiving segment then can be thought of to be coupled to this circuit as a transformer secondary. The observed in phase (representing absorption) and out of phase (representing dispersion) signals would then be proportional to the primary current and would be given by Eq. (18) and (19). Plot of out of phase signal vs. in phase signal would be a circular arc. This is the so-called DISPA plot.

A circular arc obtained in the in-phase vs. out of-phase signal plot indicates the presence of single Lorentzian line.

Presence of closely spaced lines or presence of lines with varying widths would yield distorted arcs.

2. Plots

For simplicity we consider two lines very close to each other but having different widths T_{21} and T_{22}. The DISPA plots for different ratios of T_{22}/T_{21} are shown below

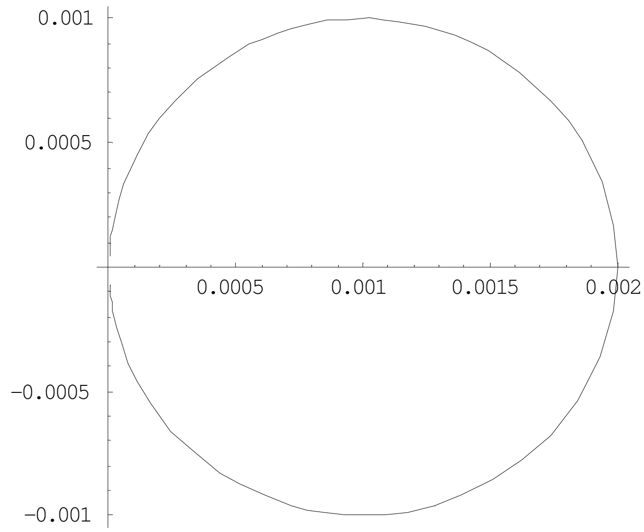

Fig 1. Plot of In Phase (Eq.18) vs. Out of Phase (Eq.19) component For $T_{22}/T_{21}=1$.

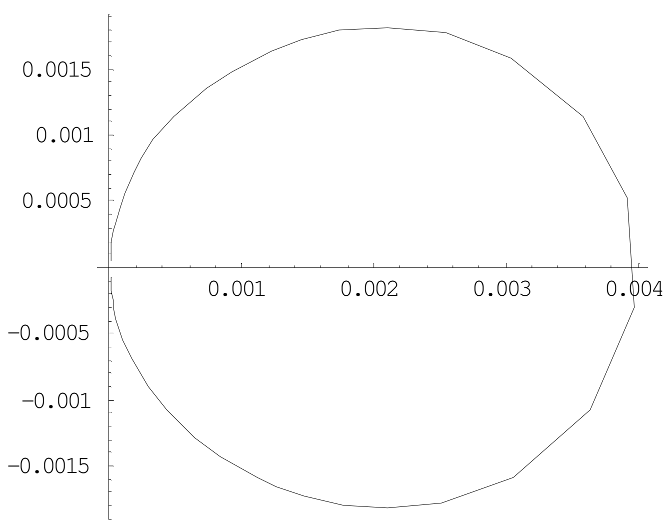

Fig 2. Plot of In Phase (Eq.18) vs. Out of Phase (Eq.19) component For $T_{22}/T_{21}=3$

3. Applications

DISPA plot of an experimentally observed line can be used to clearly indicate whether two or more lines are overlapping.

If the plot is a depressed / distorted circular arc, a High Resolution NMR run may be taken. However if a clear circular arc is obtained a High Resolution NMR scan need not be taken and NMR time may be saved.

4. Conclusion

A look at the expressions for the Bloch susceptibilities reveals that NMR phenomenon can be represented by equivalent circuit models.

Complex plane plot of out of phase vs in phase signal (the so-called DISPA plot) of a Lorenzian line yields a circle. A distorted circle in this plot indicates the presence of closely separated overlapping lines having different widths.

A DISPA plot can be used to obtain information about such lines or one may opt to go for Higher Resolution. However if such a plot is a clear circular arc higher resolution runs need not be taken and NMR time can be saved.

5. References

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