

# Estimating Field Gradients from Signal Decay Shapes

Last Revision: R. A. Schumacher March 2008  
ver. 1.5

## I. INTRODUCTION

In the NMR experiment, the “free induction decay (FID)” shape is a result of a slightly non-uniform magnetic field across the volume of the sample. In the Optical Pumping experiment, the decay of the Rabi oscillations may similarly be dominated by non-uniform magnetic field across the rubidium cell. The “decay” phenomenon seen in the two experiments is similar enough that we can discuss the physics for both at once. In both cases we can use the experimentally determined “zeros” of the decay distribution to estimate the magnetic field gradients in the samples.

## II. COMPUTING THE LINE SHAPE

The general arrangement is shown in Figure 1. Let the static magnetic field  $\vec{B}_0$  be oriented along the  $z$  axis. The spins in the sample are initially oriented along this field. The geometry of the sample is not crucial, but for discussion assume it is a cylinder of length  $L$  and cross sectional area  $A$ .

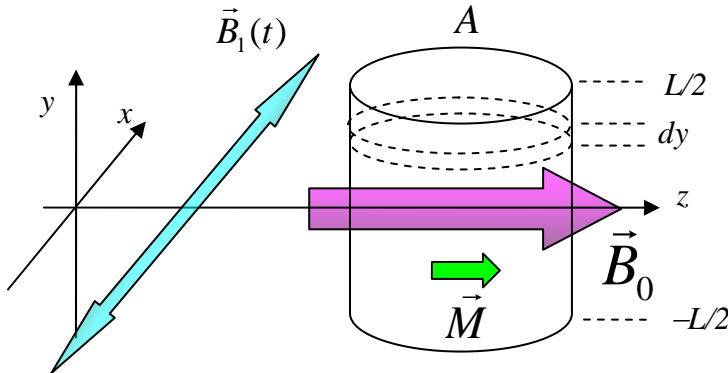


Figure 1: Let the magnetic field be in the  $z$  direction. The sample is a cylinder of length  $L$  and area  $A$ . The magnetization vector,  $\vec{M}$ , of the spins in the sample initially points along the static field  $\vec{B}_0 = B_z \hat{z}$ .

In both experiments the direction of the magnetization  $\vec{M}$  (loosely called “spin”) is changed using the same physical mechanism: a weak transverse oscillating magnetic field  $\vec{B}_1(t) = B \cos \omega_0 t \hat{x}$  is applied for some duration of time. Classically, the frequency  $\omega_0$  of this transverse RF (radio frequency) field must be matched to the Larmor frequency of the atoms in the strong static field  $\vec{B}_0$ . Given that

$$\omega_0 = \gamma |\vec{B}_0|, \quad (1)$$

where  $\gamma$  is the gyromagnetic ratio of the material under study, one can find the frequency if the field strength is known. In the NMR experiment, the frequency is near 15 MHz, while in the optical pumping experiment it is near 50 kHz. To measure a signal, in the NMR experiment we activate the oscillating field long enough to rotate the spins into the  $x$ - $y$  plane, and then observe the net magnetization in this plane as a function of time. In the optical pumping experiment, we activate the oscillating field indefinitely, sending the spin angles through many full cycles of resonance, and observe the degree of opacity of the rubidium cell versus time using a photodiode detector.

In the quantum mechanical picture, the Larmor frequency turns out to be related to the transition energy between the magnetic sub-states of the system. The splitting of the energies of the sub-states is caused the Zeeman Effect. That is, if the magnetic sub-states are separated by energy  $\Delta E$ , then we have  $\Delta E = \hbar\omega_0$ . This relationship between the quantum and classical pictures is *not obvious* at all, but comes from the study of spin and magnetic moments at the level of the Advanced Quantum Physics course. For this discussion, the classical picture is entirely sufficient.

Now suppose that the static field  $\vec{B}_0 = B_z(x, y, z)\hat{z}$  is not perfect, and that across the volume of the sample there are field gradients  $\partial B_z / \partial x$ ,  $\partial B_z / \partial y$ , and  $\partial B_z / \partial z$ . That is, in different locations in the sample the static field is slightly different, and hence the Larmor frequency is slightly different. Hence the spins precess about the static field at slightly different rates, and the coherence of the detected signal goes away after some characteristic time. That time is related to the strength of the field gradients and the size of the sample. The “line shape” of this loss of coherence is what we are calculating in this note.

For definiteness, suppose the gradient  $\partial B_z / \partial y$  is the only non-zero one we have to consider. Let the response signal of the detector to spins at location  $y_1$  be written

$$dS_1(t) = A dy \cos \omega_1 t, \quad (2)$$

and the response at a different location  $y_2$  be written

$$dS_2(t) = A dy \cos \omega_2 t, \quad (3)$$

where  $A dy$  are the separate differential volume elements across which the responses are detected.  $A dy$  is to be construed as proportional to the number of spins in the sample volume and also their net magnetization. The two  $y$  locations are not the same and can be a macroscopic distance apart. The combined response from these two locations is then

$$dS(t) = dS_1(t) + dS_2(t) = A dy (\cos \omega_1 t + \cos \omega_2 t). \quad (4)$$

Using a trigonometric identity, this is the same as

$$dS(t) = 2A dy \cos\left(\frac{1}{2}(\omega_1 + \omega_2)t\right) \cos\left(\frac{1}{2}(\omega_1 - \omega_2)t\right). \quad (5)$$

Even though the  $y$  locations can be a finite distance apart, we suppose that the frequency difference between them is still very small, so that we may write

$$\omega_1 - \omega_2 \rightarrow \Delta\omega = \gamma \Delta B_z = \gamma \frac{dB_z}{dy} (y_1 - y_2). \quad (6)$$

This equation assumes that the change in magnetic field strength across the sample is well characterized by a gradient and a separation. Put the origin at the center of the sample, and let the two locations in  $y$  be symmetric above and below  $y = 0$ , so that we have

$$\omega_1 - \omega_2 = \gamma \frac{dB_z}{dy} 2y. \quad (7)$$

For each separation of the response locations specified by  $y$ , we must include a “weighting” factor to account for all possible ways we can have two places in a sample of length  $L$  separated by distance  $2y$ . Since the sample of length  $L$ , the room within which we can place a segment of length  $2y$  is  $L - 2y$ . The dimensionless factor is taken to be  $(1 - 2y/L)$ .

We have also assumed that the spread in frequencies is so small that the bandwidth of the driving RF field is wide enough to “excite” the spins across the whole sample. If this were not the case, then only a sliver of the whole sample would respond to the oscillating magnetic field. Thus, we can define the average frequency to be equal to the driving frequency:

$$\frac{1}{2}(\omega_1 + \omega_2) \equiv \omega_0. \quad (8)$$

With these replacements we can write Eqn. (5) as

$$dS(y,t) = 2A \cos(\omega_0 t) \cos\left(\gamma \frac{dB_z}{dy} t y\right) \left(1 - 2\frac{y}{L}\right) dy. \quad (9)$$

To determine the overall response of the detector to this range of oscillatory actions within the sample we must now integrate this expression over the height of the sample. To make the integral symmetric, we will take half the result of integrating from  $-L/2$  to  $L/2$ . That is,

$$S(t) = \int dS(y,t) = A \cos(\omega_0 t) \int_{-L/2}^{L/2} \cos\left(\gamma \frac{dB_z}{dy} t y\right) \left(1 - 2\frac{y}{L}\right) dy. \quad (10)$$

Introduce, for convenience, the combination

$$k = \gamma \frac{dB_z}{dy} t, \quad (11)$$

so that we can write, with the further substitution  $\tilde{y} = k y$ ,

$$\begin{aligned} S(t) &= \int dS(y,t) = A \cos(\omega_0 t) \int_{-L/2}^{L/2} \cos(ky) \left(1 - 2 \frac{y}{L}\right) dy \\ &= A \cos(\omega_0 t) \frac{1}{k} \int \cos(\tilde{y}) d\tilde{y} + \frac{1}{k^2} \int \cos(\tilde{y}) \tilde{y} d\tilde{y} \\ &= A \cos(\omega_0 t) \frac{2 \sin k \frac{L}{2}}{k} + 0 \end{aligned} \quad (12)$$

The second integral vanishes because we are integrating an odd integrand over the symmetric range from  $-L/2$  to  $+L/2$ . This line shape function  $S(t)$  can be rewritten in a more compact form if we make the substitution

$$\Phi(t) = k \frac{L}{2} = \gamma \frac{dB_z}{dy} \frac{L}{2} t. \quad (13)$$

so that we have

$$S(t) = AL \cos(\omega_0 t) \frac{\sin \Phi(t)}{\Phi(t)} \quad (14)$$

This is our main result: it is the “line shape” of the detector response of a sample in which not all elements are oscillating at the same frequency. Note that the signal is proportional to the sample volume  $AL$ , as one would expect. At time  $t = 0$  the signal is just  $AL$ , as can be seen from the first term of the Taylor expansion of the sine. The function  $\sin \Phi / \Phi$  is the “sinc” function, which looks like a sine multiplied by a hyperbola. It has its first zero when  $\Phi = \pi$ , and then a subsequent maximum near  $\Phi = 3\pi/2$ . This is the feature we can exploit to estimate the size of the field gradient.

### III. APPLICATION TO THE NMR EXPERIMENT

In the NMR experiment, the driving frequency  $\omega_0$  is around 15 MHz, as mentioned previously, but the detector also rectifies and filters the signal so that we don't get to "see" this on the oscilloscope. Furthermore, we see the magnitude of the sinc function because the signal is rectified. This is illustrated in Figure 2.

Thus, you can try moving the sample in the magnet in the  $x$ - $y$  plane, seeking a place where the FID line shape has a zero at  $\Phi = \pi$  and a subsequent maximum near  $\Phi = 3\pi/2$ . Eqn. (13) can then be used to solve for the field gradient. If the line shape does not have this characteristic form, then the sample is probably sitting at a location where the local static field is more complicated than a smooth gradient. You will find that the gradient is very small, but evidently large enough to make free induction decay (FID) very fast relative to the quantities you are trying to measure in the experiment, namely  $T_1$  and  $T_2$ .

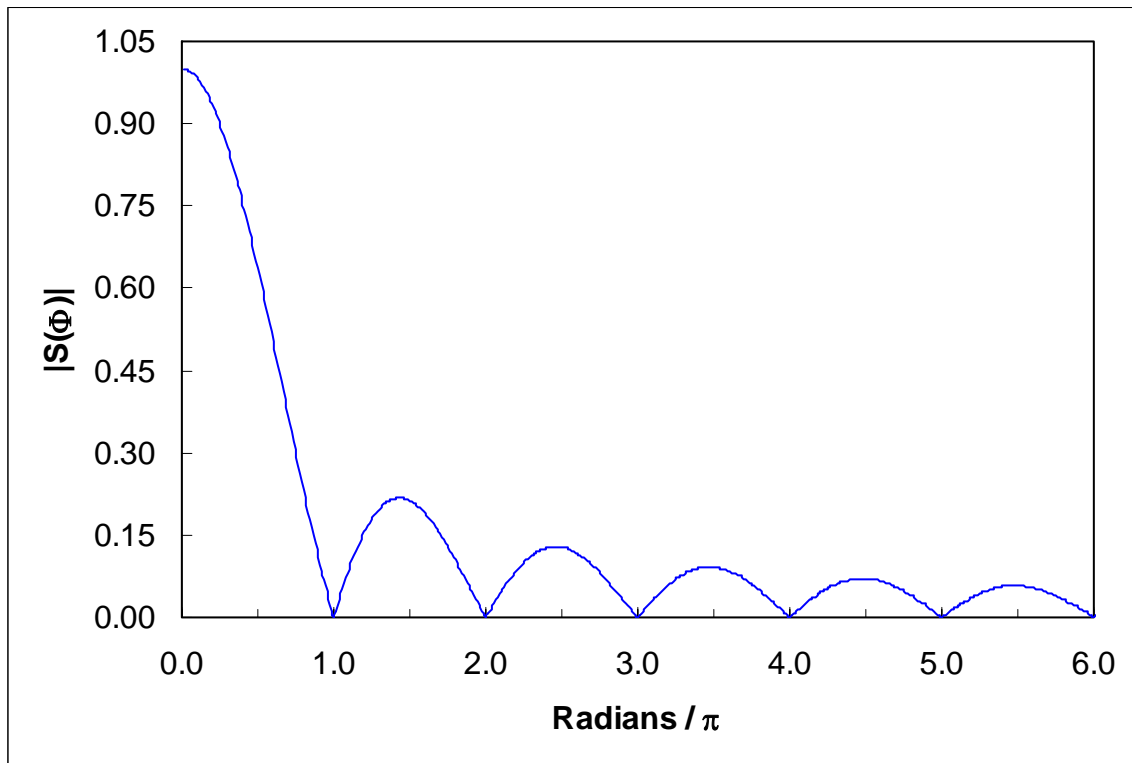


Figure 2: Simulated shape of the ideal Sinc function magnitude. The FID decay time dependence in the NMR experiment is given by this shape if the local field gradient is in the  $x$ - $y$  plane.

#### IV. APPLICATION TO THE OPTICAL PUMPING EXPERIMENT

In the optical pumping experiment the conditions are such that we see both the fast  $\cos(\omega_0 t)$  oscillation and the diminution of the strength due to the sinc function. This is illustrated in Figure 3. Trying to spot the “zero” in the sinc function at  $\Phi = \pi$  and a subsequent maximum near  $\Phi = 3\pi/2$ . It may not be easy, but you can try. Eqn. (13) can then be used to solve for the field gradient. The main difficulty is that any stray piece of ferrous metal in the vicinity of the experiment can warp the local magnetic field in a way that distorts the idealized shape shown below. You will find that this decay time is considerable faster than the other time scale in the problem, namely the time it takes the sample to get optically pumped.

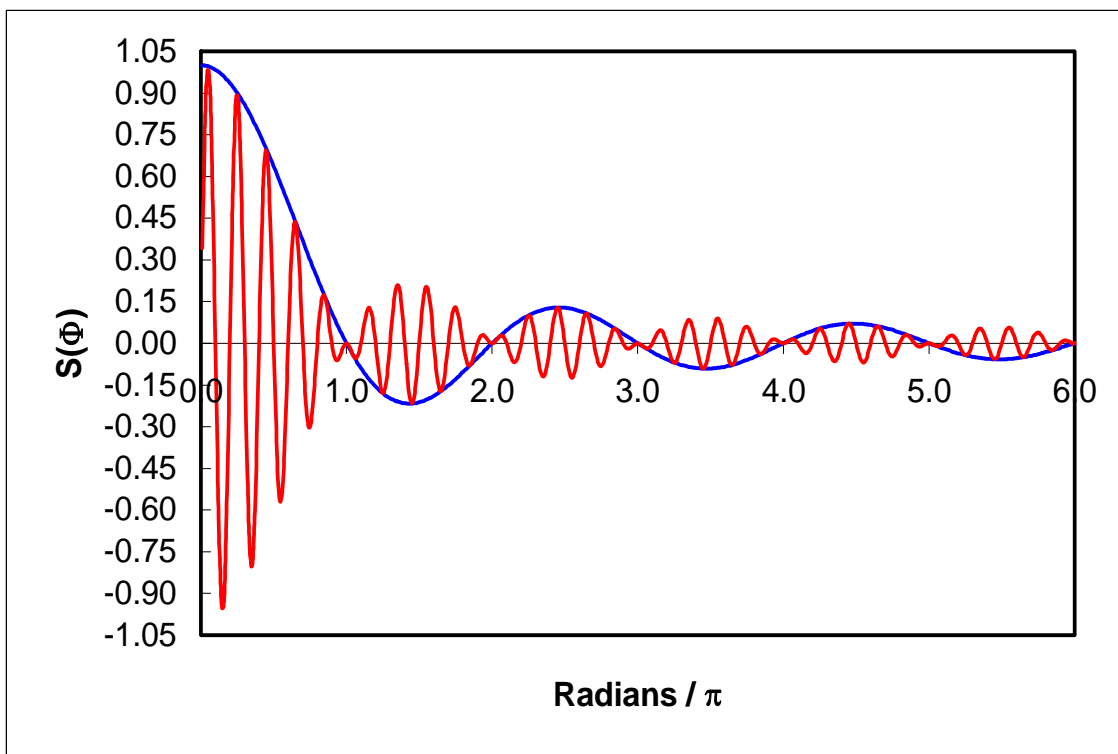


Figure 3: Simulated shape of the ideal Sinc function modulating a faster sinusoidal shape. The decay of the Rabi oscillations in the Optical Pumping experiment is given by this shape.

#### V. CONCLUSION

In conclusion, we have shown how to compute the line shape of a collection of spins that are precessing in an ambient field that is not quite “perfect” but has some gradients across the sample. By measuring the zeros of the response we can estimate the size of these gradients.