

## Theory of Radiation Damping Without the Filling Factor

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**Introduction:** The process of radiation damping is fundamental to NMR, since it describes the transfer of energy from spins to the receiver, which must occur whenever a signal is detected. However, the classic theory (1), which has served the magnetic resonance community for over 50 years, is nonetheless widely acknowledged (2,3) to contain a problematic figure of merit – the filling factor – which is difficult (if not impossible) to measure unambiguously, and for which several definitions exist in the literature. We have elsewhere shown (4) how the basic theory of the damping constant can be re-written in terms of the efficiency (5) of the probe, that is, the B1 per square root of applied power, which eliminates filling factor (and also the quality, or Q factor) from the result. We here extend that theory to cover the Bloch-Kirchhoff equations, which are transformed to a rotating frame using the methods of semiclassical laser theory, and solved numerically for some simple cases of interest in the study of DNP- hyperpolarized carbon substrates at 14.1 tesla. The new theory appears to give quantitative results for damping rates, without recourse to arbitrary scaling of the filling factor which must be drastically reduced -- to about 10% of its nominal value—to get quantitative predictions (2,3, 6).

**Theory:** The Bloch-Kirchhoff equations describing the coupling of a magnetic moment to an oscillator (e.g. a tuned coil) (1, 7) can be written in simplified form for the rotating frame as:

$$\begin{bmatrix} \ddot{M}_x \\ \ddot{M}_y \\ \ddot{M}_z \end{bmatrix} = \begin{bmatrix} -R/L & \omega_0 V B_1(1) & 0 & 0 \\ 0 & 0 & \Delta\omega & 0 \\ 0 & -\Delta\omega & 0 & \omega_1 \\ 0 & 0 & -\omega_1 & 0 \end{bmatrix} \begin{bmatrix} I \\ M_x \\ M_y \\ M_z \end{bmatrix} \quad [1.]$$

where  $I$  is the oscillator current,  $R$  and  $L$  are the coil resistance and inductance, the  $M$ 's are components of magnetization,  $V$  is the sample volume,  $\omega_0$  is the Larmor frequency,  $B(1)$  is the radiofrequency field amplitude at unit oscillator current, time differentiation is shown by dots, and other symbols follow customary usage for the Bloch equations. The simplifications of the oscillator equation follow exactly those given for a radiation oscillator in semi-classical laser theory (8). Strictly speaking, for an offset from direct resonance, a second current is required, to allow for phase shifts of the radiofrequency, but this is omitted as a needless complexity in the present formulation.

**Results and Discussion:** The simulations in the figures below were calculated with parameters corresponding to real experiments performed at 14.1 tesla, with 80 mM [1-<sup>13</sup>C] pyruvate in an 8 mm NMR tube, at a measured polarization of 7%, and a 10  $\mu$ s  $\pi/2$  pulse obtained at 164 W transmitter power. Figure 1 shows the time course, following a  $\pi/2$  pulse about the y axis, of the x magnetization, i.e. absorption mode (blue), and y magnetization, i.e. dispersion mode (green), multiplied by sample volume to give the actual magnetic moments in SI units. The z magnetization, i.e. longitudinal, is shown in red. The horizontal axis is time in seconds, and the carrier is offset from pure resonance by 10 Hz. Figure 2 gives the time course of the corresponding oscillator currents: black for absorption, and red for dispersion, which closely track the magnetizations. Figure 3 is fourier transformed spectrum, in magnitude mode, from which we estimate a linewidth of 2.5 Hz. All relaxation times are assumed to be infinite. While the basic predictions of spin dynamics do not differ from those in earlier calculations (9) damping rate in this instance is nearly quantitative, as opposed to an overestimate by an order of magnitude from the Bloembergen-Pound formulation, when translated to SI units (6)

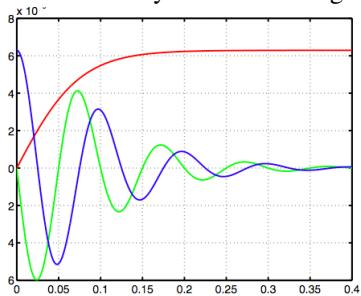


Figure 1

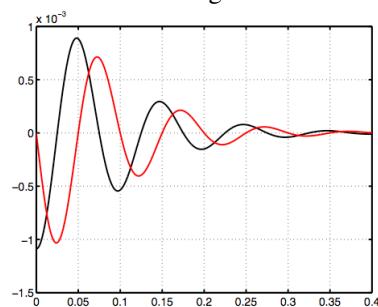


Figure 2:

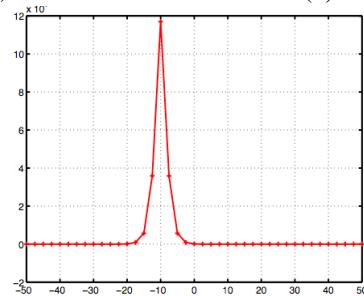


Figure 3:

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