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The NMR Reciprocity Theorem for Arbitrary Probe Geometry

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It is shown that the NMR reciprocity theorem is a variant of a problem considered by Lorentz in 1895. This formulation is quite general and applies to electric-dipole-based as well as coil-based or resonator-based magnetic resonance probes. The reasoning is related to, but different from, the proof of the reciprocity theorem for radiofrequency networks and for transmit/receive antenna systems in telecommunications. The signal-to-noise ratio of the NMR experiment is also discussed in very general terms. © 2001 Academic Press

1. INTRODUCTION

A principle of reciprocity for vibrating systems has been extensively discussed by Rayleigh (see, e.g., (*1*) and an 1873 paper cited therein). Most of his examples are mechanical, but one is about a system of wires and condensers in the presence of electromotive forces. A more general electromagnetic reciprocity relation has been given by Lorentz (*2*) and by Carson (*3*). Their work in turn has led to the reciprocity theorems for radiofrequency (rf) networks and for antenna systems.

The reciprocity theorem in NMR states that, if a given NMR probe creates a large rf magnetic field in the point R in a sample, then it has also a large sensitivity to the nuclear magnetization in R (*4*). Typical proofs (*4, 5*) assume that the "receiving" element is a loss-free coil, and apply the integral form of Faraday's induction law to the windings of the coil; for a somewhat more general approach see (*6, 7*). It is the purpose of this note to show that the reciprocity theorem holds for any "single-connector" NMR probe (excluding crossed-coil probes, which have separate connectors for transmission and detection, or MRI methods that use the whole-body coil for excitation and a local coil for detection). This is of some formal interest, because in certain applications of localized MRI the "antenna" is an electric dipole (*8*), rather than a coil. The proof is valid when the rf magnetic field is inhomogeneous in amplitude and orientation, and includes radiation and retardation effects.

The present proof of the reciprocity theorem is based on the reasoning in a 1895 paper by Lorentz (*2*). One of his intermediate results can be reformulated as a relation between the electric fields of two oscillating dipoles. Let one dipole $p_1\cos(\omega t)$ be situated in a point R_1 and another $p_2\cos(\omega t)$ in a point R_2. The medium need not be homogeneous, but has everywhere linear and isotropic relations $D = \epsilon E$ and $B = \mu H$. Let the electric fields created by these dipoles be $E_{1,2}(r)$. Then

$$p_1 \cdot E_2(R_1) = p_2 \cdot E_1(R_2). \quad [1]$$

For the NMR application, we compare the electromagnetic fields of an electric dipole (representing the transmitter as a source of rf magnetic field) and a magnetic dipole (creating a voltage at the position of the preamplifier). We will find the reciprocity relation in a form resembling $p_1 \cdot E_2(R_1) = m_2 \cdot B_1(R_2)$. We will mention briefly the relation between the NMR reciprocity theorem and the reciprocity of rf networks or telecommunication transmission/reception systems. In the final sections of this paper a general treatment is given of the ratio of signal power to noise power in the NMR spectrum.

2. MODEL

The probe, or resonator, is a spatial structure, a certain volume of which contains the sample, and which has somewhere an rf connector to the outside world. The part of the probe closest to the sample is made of a good conductor, and the coupling between the nuclear magnetism and the spectrometer occurs through currents induced on this conductor. Parts of the probe that are further away (tuning capacitor, matching networks, connector) do not couple directly to the sample, and will be considered point-like, lossless, linear, and reciprocal circuits that are not essential for the reasoning. Losses in the sample are modeled as pure ohmic losses in a poorly conducting material with a possibly high dielectric constant, as appropriate, e.g., for aqueous solutions.

Most probes manifestly use the same electromagnetic "mode" (configuration of electric and magnetic fields) for receiving and for transmitting. This is, e.g., clear when the main coupling element between the connector and the nuclear magnetization is a coil, and the windings of the coil are much closer to the sample than any other conductors. There is a rather subtle difference between the transmit and receive modes of a quadrature coil (*9*), which will show up in our equations.

In receiver mode, the fields are not derived directly from the rotating magnetic dipoles, but rather from the currents induced in the conductors by these dipoles: the boundary conditions imposed by the existence of the probe are very different from free space. In transmitter mode of course this idea of currents as source of the fields is much more direct.

We consider two situations. In the first, a point-like transmitter is hooked up to the connector, and in the second, a point-like receiver. Transmitter and receiver are modeled as one parallel-plate capacitor. In the transmitting case we suppose that the rf source is an oscillating dipole moment p between the capacitor plates, and consider the magnetic field that it creates at some point R in the sample volume. In the receiving case, the source is a rotating magnetic moment m at that point R and we look for the electric field that it creates between the capacitor plates. The transformations from the linearly oscillating dipole into a rotating magnetic field, and from the rotating magnetization into a linearly polarized electric field, will be covered by the equations developed here. (One of the mechanical examples given by Rayleigh (*1*) is the coupling between a linear and an angular displacement.)

3. MAXWELL'S EQUATIONS

A given oscillating electric polarization $P(r, t)$ is the rf field source in transmitting mode, and a rotating magnetization $M(r, t)$ is the source in receiving mode. Given these sources for the fields, we consider Maxwell's equations, without referring to a specific structure for the probe. It will be convenient to think of the "connector" as the hookup point of a tuned and matched probe (not just a coil) that will be connected through a lossless transmission line and duplexer to an actual transmitter and receiver system. From the model we have in transmitter mode (index t),

$$P_t(r, t) = p_t\delta(r)\cos(\omega t + \varphi_t) \quad [2]$$

$$M_t(r, t) = 0, \quad [3]$$

and in receiver mode (index r),

$$M_r(r, t) = m_r\delta(r - R)(\hat{x}\sin(\omega t + \varphi_r) - \hat{y}\cos(\omega t + \varphi_r)) \quad [4]$$

$$P_r(r, t) = 0. \quad [5]$$

Here p_t is an electric dipole, m_r a magnetic dipole, $\delta(r)$ a Dirac delta function, $\hat{x}$ a unit vector, the "connector" is in the origin, and the magnetic dipole is in R. The phases in Eq. [2] and Eq. [4] are with respect to some "master oscillator" (and φ_t will turn out to be unimportant).

We consider Maxwell's equations

$$\nabla \times H = j + \frac{\partial D}{\partial t} \quad [6]$$

$$\nabla \times E = -\frac{\partial B}{\partial t} \quad [7]$$

and write the constitutive equations in the form

$$H = (B/\mu_0) - M \quad [8]$$

$$D = \epsilon E + P \quad [9]$$

$$j = j^{(p)} + \sigma E. \quad [10]$$

Probe and sample are considered to have a relative permeability $\mu_r = 1$. The conductivity σ and permittivity ϵ are material properties (of the sample) that may be different in different parts of the volume of interest. Losses are supposed to be ohmic (ϵ is real). As is usual in this type of problems, the treatment is slightly different depending on whether we make the approximation of a perfect (i.e., lossless) conductor for the probe or not. In the first case, the current density on the probe $j^{(p)}$ obeys at all times

$$j^{(p)} \cdot E = 0. \quad [11]$$

In the second case we set $j^{(p)} = 0$ and introduce instead an additional probe conductivity $\sigma^{(p)}$. However, we will not write the index (p) explicitly in the following, since the probe and the sample losses clearly can be treated on equal footing.

The two sets t, r of Eq. [6] and Eq. [7] become

$$\nabla \times H_t = j_t^{(p)} + \sigma E_t + \epsilon\frac{\partial E_t}{\partial t} + \frac{\partial P_t}{\partial t} \quad [12]$$

$$\nabla \times E_t = -\mu_0\frac{\partial H_t}{\partial t} \quad [13]$$

and

$$\nabla \times H_r = j_r^{(p)} + \sigma E_r + \epsilon\frac{\partial E_r}{\partial t} \quad [14]$$

$$\nabla \times E_r = -\mu_0\frac{\partial H_r}{\partial t} - \mu_0\frac{\partial M_r}{\partial t}. \quad [15]$$

The general form of a time-harmonic field is

$$F(r, t) = F_c(r)\cos(\omega t) + F_s(r)\sin(\omega t) \qquad [16]$$

which includes the cases of linear and circular polarization. The four equations [12] to [15] now become eight equations: one set for the cos(ωt) time dependence, and another for the sin(ωt). It is usual to bring this out by introducing complex vectors (phasors) that for clarity we give the notation F and that are defined by

$$F(r, t) = \mathrm{Re}(\mathsf{F}(r)\exp(-i\omega t)) \qquad [17]$$

$$\mathsf{F}(r) = F_c(r) + iF_s(r). \qquad [18]$$

The two equations corresponding, e.g., to Eq. [14] can then be written as a single complex equation:

$$\nabla \times \mathsf{H}_r = \mathrm{j}_r^{(p)} + \sigma \mathsf{E}_r - \mathrm{i}\omega\epsilon \mathsf{E}_r. \qquad [19]$$

4. RECIPROCITY

Taking the scalar product of both sides of Eq. [12] with E_r, of Eq. [13] with H_r, of Eq. [14] with $-E_t$, of Eq. [15] with $-H_t$, and adding, we obtain

$$\nabla \cdot (E_t \times H_r - E_r \times H_t) = E_r \cdot \frac{\partial P_t}{\partial t} + B_t \cdot \frac{\partial M_r}{\partial t} + D_r \cdot \frac{\partial E_t}{\partial t} - E_t \cdot \frac{\partial D_r}{\partial t} - H_r \cdot \frac{\partial B_t}{\partial t} + B_t \cdot \frac{\partial H_r}{\partial t}. \qquad [20]$$

The terms containing the sample losses σ (and possibly probe losses $\sigma^{(p)}$) cancel; if the probe is taken as lossless, the terms containing the probe currents are zero because of Eq. [11].

Now integrate Eq. [20] over a volume that contains the origin and all points of the sample, and use the vector identity

$$\oint_{\text{surface}} (E_r \times H_t - E_t \times H_r) \cdot n dS = \int_{\text{volume}} \nabla \cdot (E_r \times H_t - E_t \times H_r) dV, \qquad [21]$$

where n is a unit vector normal to the surface element dS, pointing outward from the closed surface.

According to the experimental situation, we should make two different choices for the closed surface in the integration. If the probe is closed by a metallic screen, we take the surface of integration just outside the screen (the losses in the screen appear in Eq. [10]), where the integrand on the left-hand side of Eq. [21] vanishes. If there is no screen, as in inside-out NMR (*10*), then take the volume spherical and large enough that on its surface both the transmitter- and the receiver-mode fields behave as TEM waves arising from the origin. Then the Poynting vectors $E_t \times H_t$ and $E_r \times H_r$ both point along the normal to the surface and

$$(E_r \times H_t) \cdot n \propto (E_r \times (E_t \times n)) \cdot n = (E_r \cdot n)(E_t \cdot n) - E_r \cdot E_t \qquad [22]$$

which is symmetrical in the indices t and r, and therefore the integrand on the left-hand side of Eq. [21] is zero also in this case.

Using the definitions of P and M we obtain

$$(E_r(0, t) \cdot p_t)\sin(\omega t + \varphi_t) + m_r B_t(R, t) \times (\hat{x} \sin(\omega t + \varphi_r) - \hat{y} \cos(\omega t + \varphi_r)) = \frac{1}{\omega} \int_{\text{volume}} \left(D_r \cdot \frac{\partial E_t}{\partial t} - E_t \cdot \frac{\partial D_r}{\partial t} - H_r \cdot \frac{\partial B_t}{\partial t} + B_t \cdot \frac{\partial H_r}{\partial t} \right) dV.$$

Inserting the form of Eq. [16] it is found that the integrand in the second member is independent of time. Therefore the time-dependent parts of the first member must vanish, leaving us with two equations in terms of the scalar products of $E_{r,c}$ and $E_{r,s}$ with p_t, the scalar products of $B_{t,c}$ and $B_{t,s}$ with $m_r\hat{x}$ and $m_r\hat{y}$, and the sine and cosine functions of the phase angles φ_r and φ_t. It is easily verified that a $B_t(R, t)$ rotating in the same direction as $m_r(R, t)$ gives no time-dependent part in the scalar product $m \cdot B$ and therefore results in a linearly polarized field $E_r(0, t)$ of zero amplitude. We will come back to this later.

The general result can be obtained in a convenient compact form using phasor notation. Write the phasor analogs of Eq. [12] to Eq. [15], similar to Eq. [19], multiply with the phasors E_r, H_r, $-\mathsf{E}_t$, and $-\mathsf{E}_t$, and add the four resulting equations to obtain the analog of Eq. [20]:

$$\nabla \cdot (\mathsf{E}_t \times \mathsf{H}_r - \mathsf{E}_r \times \mathsf{H}_t) = -i\omega(\mathsf{E}_r \cdot \mathsf{p}_t \delta(r) + \mathsf{B}_t \cdot \mathsf{m}_r \delta(r - R)), \qquad [24]$$

where

$$\mathsf{p}_t = p_t \exp(-i\varphi_t) \qquad [25]$$

$$\mathsf{m}_r(R) = i(\hat{x} + i\hat{y}) m_r(R) \exp(-i\varphi_r(R)). \qquad [26]$$

The volume integral of the first member can be shown to be zero using the reasoning of Eq. [21] and Eq. [22]. Performing the volume integral of the second member, we obtain the general form of the NMR reciprocity theorem as

$$E_r(0) \cdot p_t = -B_t(R) \cdot m_r(R). \quad [27]$$

The $B_t(R)$ follow the phase angle φ_t of p_t. Therefore these phases cancel, and φ_t can be set to zero in the following.

The source of excitation p_t is linearly polarized, and therefore the simplest case is when B_t is linearly polarized as well, so that (index (l) for linear polarization)

$$B_t^{(l)}(r, t) = B_t(r)\cos(\omega t + \psi_B(r))$$
$$B_t^{(l)}(R) = \tfrac{1}{2}|B_t(R)|\exp(-i\psi_B(R))((\hat{x} + i\hat{y})\exp(-i\alpha(R)) + (\hat{x} - i\hat{y})\exp(i\alpha(R))) \quad [28]$$

where the two terms in the last equation represent two opposing rotating fields and

$$\cos(\alpha(R)) = \hat{x} \cdot B_t(R)/|B_t(R)|$$
$$\sin(\alpha(R)) = \hat{y} \cdot B_t(R)/|B_t(R)|. \quad [29]$$

The time-averaged (indicated by the overbar) energy density in the rf magnetic field is

$$\overline{B_t^{(l)}(r, t) \cdot H_t^{(l)}(r, t)} = \tfrac{1}{2}B_t^2(r)/\mu_0. \quad [30]$$

A circularly polarized $B_t^{(c)}(r, t)$ can be written as

$$B_t^{(c)}(r, t) = \tfrac{1}{2}\sqrt{2}\,|B_t(r)|(\hat{x}\cos(\omega t + \psi_B(r)) + \hat{y}\sin(\omega t + \psi_B(r)))$$
$$B_t^{(c)}(R) = \tfrac{1}{2}\sqrt{2}\,|B_t(R)|(\hat{x} + i\hat{y})\exp(-i\psi_B(R)), \quad [31]$$

where the factor $\frac{1}{2}\sqrt{2}$ has been introduced so that the energy density is $\frac{1}{2}B_t^2(r)/\mu_0$, the same as in the linearly polarized field.

The expression for $B_t^{(l)}(r, t)$ takes into account possible inhomogeneities in amplitude $B_t(r)$, in orientation in the xy plane $\alpha(r)$, and in retardation $\psi_B(r)$. After the rf pulse, the rotating nuclear magnetization will be inhomogeneous in amplitude and orientation as well. However, at each point the magnetization is in quadrature with the local phase of the pulse $(\hat{x} + i\hat{y})\exp(-i\alpha(R) - i\psi_B(R))$ so that $\varphi_r(R)$ in Eq. [4] becomes

$$\varphi_r(R) = \alpha(R) + \psi_B(R) - \pi/2 \quad [32]$$

(for a circularly polarized excitation, set $\alpha(R) = 0$).

In the model, $E_r(0)$ is the field that appears between the plates of a parallel-plate capacitor, and is linearly polarized. The direction of polarization can be taken along p,

$$E_r(0) = (p_t/|p_t|)|E_r(R)|\exp(-i\psi_E(R)), \quad [33]$$

where we write $E_r(R)$ to emphasize that the signal E_r is due to a magnetic moment (a voxel) situated in R. Given the expressions for $B_t(R)$ in Eq. [28] and for $m_r(R)$ in Eq. [26], the values of $E_r(R)$ and $\psi_E(R)$ can be found from the reciprocity theorem:

$$p_t E_r^{(l)}(R) = m_r(R)\,B_t(R)$$
$$\psi_E^{(l)}(R) = 2\psi_B(R) - \pi/2. \quad [34]$$

Note that the angle $\alpha(R)$ does not appear.

There is a subtlety in the treatment of a circularly polarized $B_t(R, t)$. If just the term in $\hat{x} + i\hat{y}$ in Eq. [31] is retained as such, the resulting value for $E_r^{(c)}$ is zero, as already mentioned in the discussion below Eq. [23]. This corresponds to the experimental fact that a quadrature coil is not a true "single-connector" device: the correct hookup is slightly different in transmit and receive modes, effectively exchanging the $\hat{x}$ and $\hat{y}$. If this change is not introduced, the detected signal is indeed zero (*9*). Incorporating this exchange into Eq. [31], we obtain

$$p_t E_r^{(c)}(R) = \sqrt{2}\,m_r(R)\,B_t(R)$$
$$\psi_E^{(c)}(R) = 2\psi_B(R) - \pi/2, \quad [35]$$

where, at constant energy density in the magnetic field, the signal has increased by a factor $\sqrt{2}$, as expected (*9*).

It is seen that retardation effects, described by the angle $\psi_E(R)$, can lead to destructive interference between the E_r coming from voxels at different R. In many cases the rf magnetic field configuration will behave similar to a cavity mode (standing, rather than travelling waves) where, apart from switching effects, retardation is unimportant. This will be assumed in the following.

A simpler form can be obtained from Eq. [34] by writing the dipole moment as $p_t = q_t d$, with q_t a charge and d the distance between the plates of the capacitor in the model; $i_t = q_t\omega$ with i_t the current in the wires between the connector and the capacitor; $E_r = \Delta\phi_r/d$ with $\Delta\phi_r$ the potential difference between the plates; and $m = M_0 V_s$, with V_s the sample volume. Then

$$\frac{\Delta\phi_r}{M_0 V_s} = \frac{\omega B_t}{i_t}. \quad [36]$$

Now $i_t\cos(\omega t + \varphi_t)$ can simply be considered the current injected into the connector during transmission, and

$\Delta\phi_r \cos(\omega t + \varphi_r)$ the voltage appearing on the connector during reception.

It is perhaps useful to stress that the reciprocity theorem takes care of all losses: by radiation (for inside-out NMR), by a finite quality factor of the coil, and by ohmic heating in the sample. So a given p will create a smaller $B_t(R)$ when any of these losses becomes more important; and the electric field $E_r(0)$ diminishes by the same factor. The proof starts from the complete Maxwell's equations, and therefore radiation and retardation effects are included, insofar as the phenomena can be described by monochromatic fields of the form of Eq. [16].

There is an interesting relation between this derivation of the NMR reciprocity theorem and the reciprocity theorem in rf network theory. The latter says that the impedance matrix for an n-port network is symmetric. Certain sources (*11*, *12*) mention a theorem due to Lorentz as the basis for the demonstration of network reciprocity. That theorem is Eq. [24], for a region of space that does not contain sources of the field,

$$\nabla \cdot (E_a \times H_b - E_b \times H_a) = 0, \qquad [37]$$

where now the indices a, b indicate two different field configurations that can exist inside the network. Imagine the network as some arrangement of microwave cavities, and the ports as waveguide flanges. The volume integral of Eq. [37] taken over the network has a bounding surface that is partly metallic, partly the waveguide apertures. The surface integral will be zero over the metallic parts. The network reciprocity theorem is then derived using

$$\sum_{\text{ports}} \iint_{\text{aperture}} (E_a \times H_b - E_b \times H_a) \cdot n dS = 0 \qquad [38]$$

as well as the relation between the fields and the impedances of the ports. For details, see, e.g., (*12*).

5. SIGNAL POWER

The reciprocity theorem is valid for idealized, loss-free structures as well as for actual probes. A really loss-free structure should be coupled to a spectrometer with infinite input and output impedances, but any practical probe can be coupled to standard transmission lines by the use of suitable impedance transformation networks. It is usually possible to construct such networks without appreciable losses of their own. The probe becomes equivalent to an idealized signal generator with an internal impedance equal to the characteristic impedance of the transmission line. Part of the signal is dissipated in the internal impedance (*13*, *14*), and an equal amount of signal power is available at the load on the other end of the transmission line. The useful signal power can therefore be calculated from the signal power dissipated in the probe.

The mechanism of dissipation is a coupling between the rotating nuclear magnetic moment m and the quadrature component (with respect to m) of the field H_r set up by the j_r induced by that same magnetic moment. In a loss-free probe, the component of $B_r(t)$ that rotates at $+\omega$ is parallel to $M_r(t)$, and does not reorient that magnetization. According to Lenz's law, it compensates exactly the changing flux due to $M_r(t)$: $B_{r,\parallel} = \mu_0(H_{r,\parallel} + M_r) = 0$.

When losses are taken into account, there will appear a current density in phase with the electric field, generating an $H_r(t)$ in quadrature with $M_r(t)$. Denoting this component by $H_{r,\perp}$

$$\begin{aligned} B_r \cdot H_r &\approx \mu_0(H_{r,\parallel} + M_r + H_{r,\perp}) \cdot (H_{r,\parallel} + H_{r,\perp}) \\ &= \mu_0 |H_{r,\perp}|^2. \end{aligned} \qquad [39]$$

The torque exerted by $H_{r,\perp}$ drives the magnetization back to the static field B_0. The magnetic energy $m \cdot B_0$ so gained is dissipated in the probe losses and in the detector.

The losses in the probe and in the sample can be characterized by the quality factor Q of the "resonator mode" with the sample in place. Quite generally, the inductance L of the probe is defined as

$$\tfrac{1}{2} L i_t^2 = \int_{\text{space}} \overline{B_t(r, t) \cdot H_t(r, t)} dV, \qquad [40]$$

where the overbar indicates a time average over a cycle, and i_t is the amplitude of a sinusoidal current input into the connector. The integral is taken over the space occupied by the probe (including matching networks, etc., but excluding the transmitter itself) and the sample. Similarly, the equivalent loss resistance R of the probe with sample is

$$\tfrac{1}{2} R i_t^2 = \int_{\text{space}} \sigma(r) \overline{E_t(r, t) \cdot E_t(r, t)} dV. \qquad [41]$$

The value of Q is defined as $Q = \omega L/R$. The filling factor η is by definition the fraction of the magnetic field energy stored in the sample volume,

$$\eta Q = \frac{\omega \int_{\text{sample}} \overline{B(r, t) \cdot H(r, t)} dV}{\int_{\text{space}} \sigma(r) \overline{E(r, t) \cdot E(r, t)} dV} = \frac{\omega \int_{\text{sample}} B^2 dV}{2\mu_0 P^{(p)}}, \qquad [42]$$

where all losses have been supposed in the sample and probe and $P^{(p)}$ is the corresponding power. In principle, we must distinguish the receiver mode $(\eta Q)_r$ and the transmitter mode $(\eta Q)_t$, but we will see below that the reciprocity theorem implies that the two are equal.

In an impedance-matched system consisting of a power source (the probe with sample in place), a lossless transmission line, and a detector (the preamplifier), the power dissipated in the detector $P^{(d)}$ equals that dissipated in the source $P^{(p)}$,

$$\begin{aligned} 2P^{(p)} &= P^{(d)} + P^{(p)} \\ &= \frac{d}{dt}\int_{\text{sample}} M_r(r,\,t)\cdot B_0 dV \\ &= \gamma \int_{\text{sample}} (M_r(r,\,t)\times B_r(r,\,t))\cdot B_0 dV \\ &= \tfrac{1}{2}\,\omega \int_{\text{sample}} M_r B_r dV, \end{aligned} \quad [43]$$

where the factor $\frac{1}{2}$ in the last member is for a linearly polarized $B_r(r,\,t)$; for a circularly polarized field it is $\frac{1}{2}\sqrt{2}$; compare Eq. [28] and Eq. [31]. (The factor $\frac{1}{2}$ is missing from Eq. [10] in (*15*), and as a consequence the signal-to-noise ratio in that paper is 6 dB too high.)

If the amplitudes M_r and B_r are reasonably uniform over the sample volume V_s then, according to Eq. [42] for $(\eta Q)_r$ and Eq. [43], the signal power arriving at the detector immediately after a $\pi/2$ pulse ($M_r = M_0$) is (*15*)

$$\begin{aligned} P_r^{(d)} &= \frac{\omega^3}{8\mu_0}(\eta Q)_r\left(\frac{\chi_0}{\gamma}\right)^2 V_s \\ &= \tfrac{1}{4}\mathcal{M}B_0\tau_{\text{rad}}^{-1}, \end{aligned} \quad [44]$$

where χ_0 is the nuclear magnetic susceptibility, $\mathcal{M} = \chi_0 B_0 V_s/\mu_0$ is the total nuclear magnetic moment of the sample, and $\tau_{\text{rad}}^{-1} = \frac{1}{2}\chi_0\omega(\eta Q)$ is the inverse time constant for decay of the signal through radiation damping (*16*). For a circularly polarized $B_r(r,\,t)$, the right-hand side must be multiplied by 2.

We can also calculate $P_r^{(d)}$ from the definition of $(\eta Q)_t$ for a homogeneous rf field

$$(\eta Q)_t = \frac{V_s}{\mu_0\omega R}\left(\frac{\omega B_t}{i_t}\right)^2 \quad [45]$$

and the reciprocity theorem in the form of Eq. [36]. In a matched system, the voltage $\Delta\phi_r$ appears across a resistance $2R$. Then

$$2P_r^{(d)} = \frac{\frac{1}{2}(\Delta\phi_r)^2}{2R} = \frac{1}{4R}\left(\mathcal{M}\,\frac{\omega B_t}{i_t}\right)^2 = \frac{\mu_0}{4V_s}(\eta Q)_t\omega\mathcal{M}^2 \quad [46]$$

while, for a homogeneous (and linearly polarized) B_t, we have from Eq. [42] and Eq. [36]

$$(\eta Q)_t = \frac{V_s}{\mu_0\omega R}\left(\frac{\omega B_t}{i_t}\right)^2 = \frac{V_s}{\mu_0\omega R}\left(\frac{\Delta\phi_r}{M_o V_s}\right)^2. \quad [47]$$

Comparison of Eq. [46] and Eq. [44] shows that the reciprocity theorem may also be stated as

$$(\eta Q)_r = (\eta Q)_t. \quad [48]$$

Substitution of Eq. [45] and Eq. [48] into Eq. [44] yields the result in Eq. [17] of Haeberlen's summer school notes (*5*).

6. SIGNAL-TO-NOISE RATIO

In a matched system of characteristic impedance R the rms noise voltage generated by the source in a frequency range $\Delta\nu = \Delta\omega/2\pi$ is $2(kTR\Delta\nu)^{1/2}$. Half of this voltage appears across the detector and therefore the noise power coming from the probe, and available after a unity-gain detector system with an ideal low-pass filter of bandwidth $\Delta\omega \ll \omega/Q$, is

$$P^{(n)}(t) = kT\,\frac{\Delta\omega}{2\pi}. \quad [49]$$

The signal-to-noise power ratio varies with temperature as T^{-3}, if it can be assumed that the noise source is at the same temperature as the sample, and Q is independent of temperature. (Actually, the basic derivation of Eq. [49] involves equilibrium thermodynamics: strictly speaking, noise source and detector must be at the same temperature). From Eq. [44], Eq. [47], and Eq. [49] we find the same signal-to-noise ratio as from Eq. [4] and Eq. [6] in (*4*). It follows from Eq. [44] and Eq. [49] that Eq. [38] of (*17*), which has been derived for small flip angles, is in fact valid for arbitrary angles.

The variation of $P^{(d)}/P^{(n)}$ with field depends on the factor $(\eta Q)\omega^3$. If the sample is an aqueous solution, and currents associated with the electric fields created according to Eq. [13] dominate the quality factor, then $Q \propto \omega^{-1}$. This effect is usually important in MRI (*18*). At a given field, temperature, sample or voxel volume, and (if in the time domain) bandwidth, the signal-to-noise ratio can *only* be improved by optimizing the parameter ηQ.

For the case of MRI, the index "sample" on the integral in Eq. [42] should be changed to "voxel" and the index "space" to "body," since now the losses will be through σ(body). An algorithm, based on this criterion for $(\eta Q)_t$, to determine the "ultimate signal-to-noise ratio" for a given voxel inside a lossy elliptical cylinder has been proposed in (*19*). As a rule, not all voxels can be optimized simultaneously by one and the same coil design.

Of course, as the time t after the $\pi/2$ pulse increases, the signal power decreases. Assume for simplicity a simple exponential decay with time constant $T_2^*/2$

$$P_r^{(d)}(t) = P_r^{(d)}(0)\exp(-2t/T_2^*) \quad [50]$$

with $P_r^{(d)}(0)$ given by Eq. [44] or Eq. [46]. If the signal trace is recorded during an interval t_m, the average signal power $\bar{P}_r^{(d)}$ is

$$\bar{P}_r^{(d)} = \frac{P_r^{(d)}(0)}{t_m}\int_0^{t_m} \exp(-2t/T_2^*)dt. \quad [51]$$

After Fourier transformation approximately two-thirds of this power appears in a frequency window covering the half-width of the absorption lineshape $\Delta\omega = 2/T_2^*$. Inside this window the average signal-to-noise power ratio is

$$(S/N)_{\Delta\omega} = \frac{2\pi T_2^* \bar{P}_r^{(d)}}{3kT}. \quad [52]$$

In high-resolution liquids NMR or in MRI the lineshape usually does not convey interesting information, and it is desirable to apply a digital filter to enhance the signal-to-noise ratio. The filter should conserve the value of $P_r^{(d)}(0)$, since this is proportional to the number of nuclei, but it may alter the effective value of T_2^*. Consider the Lorentzian convolution that consists in multiplying the (two channels of the complex) FID signal $f(t)$ with $\exp(-t/T_2^*)$, $0 < t < t_m$, creating a "filter output" $f_o(t)$. This halves the effective value of T_2^* in the expression for the signal power, Eq. [50]. To see the effect on the noise, consider the autocorrelation $R_o(\tau)$ of $f_o(t)$ when the input is noise $n(t)$, white from $-\omega_c$ to ω_c, with an autocorrelation

$$\langle n(t)n(t+\tau)\rangle = \langle n^2(t)\rangle \frac{\sin(\omega_c\tau)}{\omega_c\tau}. \quad [53]$$

The output autocorrelation function is

$$R_o^{(n)}(\tau) = \lim_{T\to\infty}\frac{1}{T}\int_{T_1}^{T_1+T} n(t)n(t+\tau)\exp(-(2t+\tau)/T_2^*)dt$$
$$\approx \frac{1}{t_m}\int_0^{t_m} n(t)n(t+\tau)\exp(-(2t+\tau)/T_2^*)dt$$
$$= \langle n(t)n(t+\tau)\rangle\exp(-\tau/T_2^*) \times \frac{1}{t_m}\int_0^{t_m}\exp(-2t/T_2^*)dt. \quad [54]$$

After Fourier transformation, the noise power in a frequency interval $\Delta\omega$ is $P_o^{(n)}(\omega)\Delta\omega$ with

$$P_o^{(n)}(\omega) = \frac{kT}{2\pi}\frac{1}{t_m}\int_0^{t_m}\exp(-2t/T_2^*)dt \times \pi^{-1}(\arctan(\omega_c T_2^* - \omega T_2^*) + \arctan(\omega_c T_2^* + \omega T_2^*)). \quad [55]$$

For $\omega_c T_2^* \gg 1$ and near the center of the spectrum, where $\omega T_2^* < 1$, the noise power is independent of frequency. The signal-to-noise power ratio becomes

$$(S/N)_o = \frac{\pi T_2^* P_r^{(d)}(0)}{6kT}(1 + \exp(-2t_m/T_2^*)). \quad [56]$$

If the lifetime of the free induction decay signal is determined by radiation damping, then $T_2^* = \tau_{\text{rad}}$, and a lower Q will give the same signal-to-noise ratio, because of Eq. [44]. Although it is not of much practical interest, the ultimate $(S/N)_o$ in this limit of very high ηQ is seen to be

$$(S/N)_o^{\text{ult}} = \frac{\pi}{24}\frac{\mathcal{M}B_0}{kT} \quad [57]$$

and the signal-to-noise ratio in the half-width of the line in the absorption spectrum is proportional to B_0/T.

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