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Local measure of the electromagnetic field in magnetic resonance coils: How do simulations help to disentangle the contributions of the electric and magnetic fields?

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ABSTRACT

The development of probes for Nuclear Magnetic Resonance (NMR) spectroscopy of metabolites, biomolecules or materials requires the accurate determination of the radio-frequency (RF) magnetic field strength, B_1, at the position of the sample since this RF-field strength is related to the signal sensitivity and the excitation bandwidth. The Ball Shift (*BS*) technique is a commonly employed test bench method to measure the B_1 value. Nevertheless, the influence of the RF electric field, E_1, on *BS* is often overlooked. Herein, we derive, from Maxwell equations, an analytical expression of the *BS*, which shows the contribution of both the electric and magnetic energies to the *BS* value. This equation shows that the *BS* allows quantifying the B_1 field strength only in regions where the electric energy is small with respect to the magnetic one. The numerical simulations of electromagnetic (EM) field and energy prove that this condition is fulfilled at 100.5 MHz inside the electrically balanced coil of a double-resonance ^{1}H/X 4 mm Magic Angle Spinning (MAS) probe since for that circuit, the center of the coil is an antinode for the B_1 standing wave and a node for the E_1 one. We also show that the simulated *BS* values agree well with the experimental ones. Conversely, NMR experiments show that the contribution of the electric energy to *BS* becomes significant when the X channel of this probe is connected to a frequency splitter. In that case, the use of *BS* method to estimate the B_1 value is compromised.

1. Introduction

Nuclear Magnetic Resonance (NMR) experiments are currently used in numerous fields, including medical imaging, chemistry, physics, materials science, structural biology, food science, oil exploration as well as heritage science [1–6].

NMR linear experiments are carried out by placing the investigated sample in an external static magnetic field, B_0, and by applying a linearly oscillating magnetic field, B_1, at a radio-frequency (RF) close to the Larmor frequency of the detected isotope ($\omega_0 = -\gamma B_0$ where γ is the nuclear gyromagnetic ratio). The design of NMR instrumentation requires reliable and fast optimization of the probe efficiency, $B_1/\sqrt{P}$, with P being the transmitter power, since: (i) according to the reciprocity principle, the NMR sensitivity is proportional to this efficiency [7], (ii) high power can cause arcing and electric instabilities, and (iii) large B_1 strength increases the excitation bandwidth in pulsed NMR experiments.

A first simple method to measure B_1 consists in acquiring a nutation curve, i.e. the intensity of the NMR signal as function of the pulse length in the pulse-acquire experiment since the nutation frequency of the nuclear magnetization around the B_1 field is proportional to γB_1 [8–10]. However, this measurement requires the use of an NMR spectrometer. Such equipment is expensive and the available measurement time is often limited on these spectrometers, especially for those operating at high magnetic field. Therefore, the nutation curve method is not well-suited for the prototyping of NMR instrumentation. Moreover, nutation curves only provide the distribution of B_1 field in the frequency space. The dependence of B_1 on the spatial position requires (i) the measurement of nutation curves of small-size samples placed at different locations in the detection coil (hereinafter referred to as the coil) [11,12], or (ii) the acquisition of two-dimensional (2D) nutation experiments in the presence of strong magnetic field gradients

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[13]. In practice, these experiments are mainly applicable for sensitive isotopes, such as ^{1}H.

The performances of the RF circuit of an NMR probe can be easily estimated by measuring its quality factor (Q). This figure of merit characterizes the ability of the RF circuit to store energy at its resonance frequency. The Q factor corresponds to the frequency-to-bandwith ratio of the resonance in the reflection curve and hence can be easily estimated using a network analyzer. Nevertheless, the Q factor is measured at the entrance of the probe and hence it does not permit discerning between the RF magnetic energy stored either in the coil producing B_1 field or in other parts of the probe. In other words, high Q factors can be measured even if the B_1 field is low.

The pickup coil is a commonly employed bench tool providing the direct measurement of the B_1 field strength [14,15]. This method does not require the use of an NMR spectrometer. Furthermore, contrary to the nutation experiment, it does not involve the detection of the NMR signal and hence it is applicable for insensitive nuclei. Pickup coils are widely used to estimate the B_1 field produced by surface coils or large volume resonators. Nevertheless, they are less suitable to measure the B_1 field at the center of a solenoid since such measurement requires small pickup coils, which are difficult to build and to align properly.

Another bench tool to estimate the B_1 field strength is the *Ball Shift* (*BS*) technique [16,17]. It consists in measuring the shift of the tuning frequency of the electronic circuit producing the B_1 field when a metallic conductor, often a sphere or a disk, is placed at the position of the sample (see Fig. 1). For solid-state NMR probes, the *BS* is often measured as the change in tuning frequency between a rotor containing a conductor and an empty one. As small metal spheres are easier to build and to position than small coils, the *BS* method is more suitable than the pickup coil in the case of solenoids or other resonators with small active volumes. The *BS* method has notably been used to map the inhomogeneity of the B_1 field in NMR coils or Electron Paramagnetic Resonance (EPR) resonators [14,18–20]. This method assumes that the *BS* is proportional to the square of the B_1 field at the position of the ball.

Nevertheless, it has been reported that the *BS* method cannot measure simultaneously the electric and magnetic fields, which are concomitant in NMR coils and EPR resonators [17]. Therefore, when quantifying the B_1 strength using the *BS* method, it is important to estimate the electric field value, E_1. Experimentally, this can be done by the dielectric shift (*DS*) method that consists in measuring the change in the tuning frequency of the electronic circuit when a dielectric material is placed inside the coil. For solid-state NMR probes, such dielectric insert is often the empty rotor used to measure the *BS*. The *Magnetic to Electric Ratio* ($MER = -BS/DS$) allows estimating the relative strength of B_1 and E_1 fields.

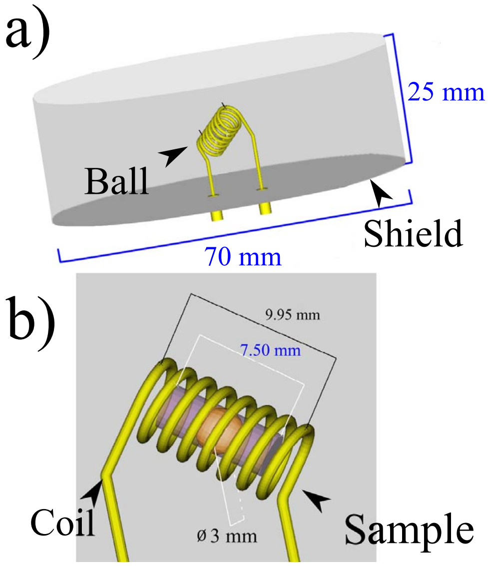

Fig. 1. (a) Cavity used for the EM simulation. For the sake of readability, the rotor is not shown in (a) and (b). The expansion of the upper figure showing the coil (b), the metal ball, and the sample volume as a cylinder. Additional details are given in the Section 3.

When the coil is perfectly balanced in the circuit, B_1 and E_1 fields are maximal and minimal, respectively, at the center of the coil [20–24]. In that case, high *MER* values are measured and the *BS* method provides reliable B_1 values. Unfortunately, to the best of our knowledge, there is a lack of detailed study to estimate how the electric field E_1 influences the *BS* values. The advent of softwares for the simulation of electromagnetic (EM) fields offers new possibilities to investigate this question [25]. These softwares allow calculating realistic dependences of the EM field with the position inside an NMR probe [23,26]. Furthermore, contrary to approaches based on the Biot-Savart law, which is only valid in the magnetostatic approximation [8,27,28], these softwares provide reliable numerical solutions of Maxwell equations at high frequencies, in cases for which effects originating from the propagation of EM waves within the NMR probe must be taken into account. The aim of this work was to derive an analytic function for the *BS* and to investigate the conditions of validity of the *BS* measurement using full wave electrodynamic simulations and experiments.

2. Theory

We consider a resonator of initial volume Ω_a contained within a Gaussian surface, Σ_a, as depicted in Fig. 2a. The Ω_a volume contains dielectric materials, such as air or the rotor. The permittivity, ϵ, depends on the position because it differs between the air and the rotor walls. Conversely, the difference of permeability, μ, between the air and the rotor walls is small (about 1 ppm between air and zirconia) and is neglected hereafter. The walls of the cavity are assumed to be Perfect Electric Conductors (PEC), i.e. they exhibit zero resistivity. For a cavity containing a coil, such as that shown in Fig. 1, the Σ_a surface includes the surface of the coil. The cavity operates in the sinusoidal steady-state regime and the phasors of the RF electric and magnetic fields inside the cavity are denoted by $\mathbf{E}_{1a}$ and $\mathbf{B}_{1a}$. In the following, we also consider the phasor of the magnetizing field $\mathbf{H}_{1a} = \mathbf{B}_{1a}/\mu$. The resonance frequency of this resonator is denoted ν_a.

In the *BS* measurement, we introduce in the above resonator a PEC ball with a volume $\Delta\Omega$ and an outer surface $\Delta\Sigma$ (see Fig. 2b). Hence, the volume of vacuum in the resonator is decreased to $\Omega_b = \Omega_a - \Delta\Omega$ and the Gaussian surface of this volume becomes: $\Sigma_b = \Sigma_a \cup \Delta\Sigma$. During perturbation by the ball, the different physical quantities are labeled with the subscript b. In particular, the ball shifts the resonance frequency, which becomes $\nu_b = \nu_a + \Delta\nu_{BS}$ with $\Delta\nu_{BS}$ the *BS* value. In the appendix, we derive from Maxwell equations an analytical expression of $\Delta\nu_{BS}$ as function of $\mathbf{E}_{1i}$ and $\mathbf{H}_{1i}$ with i=a or b:

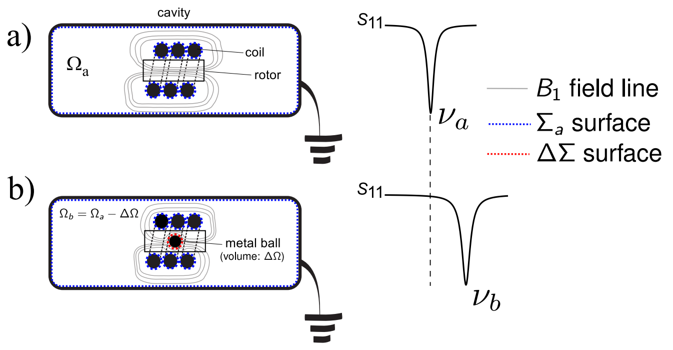

Fig. 2. Schemes describing the *BS* method as well as the volumes and the surfaces considered in the Section 2. (a) The cavity containing the sample coil and an empty rotor resonates at the frequency ν_a, as seen in the reflection curve shown on the right-hand side of the subfigure. (b) Replacing the empty rotor by a rotor containing a metal ball shifts the resonance frequency of the cavity to ν_b.