

Feedback schemes for radiation damping suppression in NMR: A control-theoretical perspective

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ABSTRACT

In Nuclear Magnetic Resonance (NMR) spectroscopy, the measurement of the collective spin magnetization is weakly invasive and its back-action is called radiation damping. The aim of this paper is to provide a control-theoretical analysis of the problem of suppressing radiation damping effects. We show that the various real-time feedback schemes commonly used in NMR can be cast in terms of high gain feedback, of exact cancellation based on knowledge of the radiation damping field, and of 2-degree of freedom control designs, with the exact cancellation as prefeedback. We further show that the formulation in control-theoretical terms naturally leads to devising other possible closed-loop schemes, such as a general high gain feedback stabilization design not requiring the knowledge of the radiation damping field.

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1. Introduction

Nuclear Magnetic Resonance (NMR) has achieved an exceptional degree of control on the dynamics of quantum spin systems, through the development of techniques such as shaped pulses, composite pulses, refocusing schemes, and effective Hamiltonians (see for example [1–3] for a review of NMR and [4,5] for some more advanced control strategies). These control techniques allow for the precise spectroscopy of complex molecules by compensating for experimental systematic errors and departures of the real systems from ideal, simplified models. Most of these control techniques are based on open loop control, contrary to the practice in most other domains where control is based on closed loop and feedback. An instance of application of feedback in NMR is given by techniques for reducing the effects of radiation damping.

Radiation damping is a phenomenon occurring in an NMR spectrometer in the presence of a collective spin measurement [6–8]. During a measurement, the nuclear spins precess about the external magnetic field, inducing an oscillating current in the detection coil that creates an electromagnetic field. This field in turn interacts with the spins in the sample, inducing a back-action on the system observed. In high field and probes of a high quality factor, radiation damping is typically an important effect only at certain frequency

ranges, for example that of the abundant spin of the solvent. At these frequencies, it behaves much like a soft pulse, steering the magnetization vector back to its thermal equilibrium direction. In other situations the back-action signal is so weak that it is dominated by the relaxation effects, and hence it is negligible. In order to focus on the radiation damping effects only, in this work we assume to be dealing with one of those situations in which radiation damping is of interest, and it is comparable or dominates over relaxation effects.

A model of radiation damping has existed since the fifties [6,7], and assumes that the back-action is conservative, i.e., it preserves the norm of the Bloch vector. Efforts to engineer the NMR receiving/transmitting system in order to reject this form of back-action have been carried out for more than a decade. Many strategies to compensate for radiation damping have been devised, such as electronic feedback [9–12], rf pulse compensation [13], gradient field, Q-switches, and composite pulse sequences, see [8,12] for more detailed surveys. We are here interested only in the first two methods.

The aim of this paper is threefold. First, we provide a rigorous convergence analysis of the behavior induced by the radiation damping effect and described qualitatively in several papers [14,15,8,16,17]. Second, we aim to give a system-theoretic interpretation of the electronic feedback and pulse compensation control designs found in the NMR literature. In the so-called “Ecole Polytechnique design” [12], the compensation scheme can be thought of as an exact feedback matching problem, i.e., a precompensator based on the knowledge of the radiation damping field

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deriving from the accepted model of radiation damping. In the presence of uncertainty in the radiation damping field knowledge (or in the model leading to the evaluation of its value), a high gain variant of the same control problem can be set up in order to maintain the spin in the “fully inverted” state. This scheme however only works for this particular state; for generic states, the exact cancellation of the radiation damping alone does not achieve asymptotic stabilization. However, the precompensator can still be intended as a prefeedback to which a second active field can be linearly superimposed, in order to produce desired control actions. In control terms, this design is called a 2-degrees of freedom (DOF) control design, and resembles the schemes described in [13,12].

The third and last aim of this paper is to explore possible alternative/improved schemes inspired by control theory. In the spirit of feedback control, we show that the 2-DOF design mentioned above can be completed with an extra feedback loop, allowing to achieve closed-loop asymptotic stabilization, a more robust concept than just exact canceling by matching. We will further see that also a high gain state feedback can be designed in order to achieve tracking of a desired trajectory up to a limited steady state tracking error. Unlike the 2 DOF scheme based on exact radiation damping cancellation, this last feedback controller does not require the explicit knowledge of the radiation damping field. For “high gain” we mean a ratio of around an order of magnitude between the actuation current and the current produced by the spin precession. Hence the task of radiation damping compensation can be performed in the soft pulse regime, meaning that real-time feedback makes sense in this context even with a single coil available. When strong pulses are instead considered, the transmitter/receiver ratio is several orders of magnitude higher, hence alternative designs such as, for example, an interleaved scheme of pulsing and measuring, should be used instead.

2. The model for radiation damping

In the following, we shall consider the model of radiation damping described e.g. in [6–8,15,18], focusing only on the spin 1/2 case. Further details concerning the model formulation are available in the [Appendix](#).

Disregarding relaxation effects (i.e., when the relaxation time constants [1] tend to infinity: $T_1 = T_2 = \infty$) and denoting with $\mathbf{m} = [m_x \ m_y \ m_z]^T$ the normalized Bloch vector, ($\mathbf{m} = \mathbf{M}/M_0$ where M_0 is the equilibrium magnetization), the nonlinear Bloch equations for radiation damping in a frame rotating with the circuit resonant frequency are

$$\begin{aligned} \frac{dm_x}{dt} &= \delta m_y - \ell m_x m_z \\ \frac{dm_y}{dt} &= -\delta m_x - \ell m_y m_z \\ \frac{dm_z}{dt} &= \ell(m_x^2 + m_y^2) \end{aligned} \quad (1)$$

where $\delta = \omega - \omega_0$ is the offset between the Larmor precession frequency ω_0 and the circuit resonant frequency ω , ℓ is the radiation damping rate $\ell = \frac{1}{T_R}$, with T_R the radiation damping time constant $T_R = \frac{\gamma}{2\pi\xi M_0 Q}$ (γ = gyromagnetic ratio, ξ = coil filling factor, Q = probe quality factor) [7,8,15]. Denoting A_x, A_y and A_z the real rotation matrices respectively around the x, y , and z axis,

$$\begin{aligned} A_x &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, & A_y &= \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \\ A_z &= \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \end{aligned}$$

for which $\text{Lie}(A_x, A_y, A_z) = \text{span}(A_x, A_y, A_z) = \mathfrak{so}(3)$, then (1) can be written as

$$\frac{d\mathbf{m}}{dt} = -\delta A_z \mathbf{m} + \ell \langle \langle \mathbf{m}_0, A_x \mathbf{m} \rangle \rangle A_x \mathbf{m} + \ell \langle \langle \mathbf{m}_0, A_y \mathbf{m} \rangle \rangle A_y \mathbf{m} \quad (2)$$

where $\mathbf{m}_0 = [0 \ 0 \ 1]^T$ is the north pole of the Bloch sphere (aligned with the static magnetic field applied to the ensemble) and $\langle \langle \cdot, \cdot \rangle \rangle$ denotes a Euclidean inner product in \mathbb{R}^3 .

Proposition 1. *The system (2) has \mathbf{m}_0 as an almost globally asymptotically stable equilibrium point, with region of attraction $\mathbb{S}^2 \setminus \{\mathbf{m}_1\}$, where $\mathbf{m}_1 = [0 \ 0 \ -1]^T$ is the inverted state.*

Proof. Consider the \mathbb{S}^2 -distance

$$V = \|\mathbf{m}\|^2 - \langle \langle \mathbf{m}_0, \mathbf{m} \rangle \rangle. \quad (3)$$

Clearly $V(\mathbf{m}) > 0 \ \forall \mathbf{m} \in \mathbb{S}^2 \setminus \{\mathbf{m}_0\}$, $V(\mathbf{m}_0) = 0$. Differentiating along the trajectories of (2):

$$\begin{aligned} \dot{V} &= -\langle \langle \mathbf{m}_0, \dot{\mathbf{m}} \rangle \rangle = \delta \langle \langle \mathbf{m}_0, A_z \mathbf{m} \rangle \rangle - \ell \langle \langle \mathbf{m}_0, A_x \mathbf{m} \rangle \rangle \langle \langle \mathbf{m}_0, A_x \mathbf{m} \rangle \rangle \\ &\quad - \ell \langle \langle \mathbf{m}_0, A_y \mathbf{m} \rangle \rangle \langle \langle \mathbf{m}_0, A_y \mathbf{m} \rangle \rangle. \end{aligned}$$

Since $A_z \mathbf{m}_0 = [0 \ 0 \ 0]^T$, the first term disappears and hence

$$\dot{V} = -\ell \langle \langle \mathbf{m}_0, A_x \mathbf{m} \rangle \rangle^2 - \ell \langle \langle \mathbf{m}_0, A_y \mathbf{m} \rangle \rangle^2 \leq 0.$$

Therefore $V(\cdot)$ is a Lyapunov function for the equilibrium \mathbf{m}_0 of (2). As $\dot{V} = 0$ only for $\mathbf{m} = \mathbf{m}_0$ or $\mathbf{m} = \mathbf{m}_1$, \mathbf{m}_0 is an attractor for (2) with basin of attraction $\mathbb{S}^2 \setminus \{\mathbf{m}_1\}$. \square

It is straightforward to check that the inverted state \mathbf{m}_1 is an unstable equilibrium of (2). In fact, in the literature, it is known that a weak perturbation or even a noise disturbing \mathbf{m} can trigger the coherent radiation from \mathbf{m}_1 to the lower energy state \mathbf{m}_0 [17,16].

3. Feedback control strategies

For a coil aligned for instance with the laboratory x axis, the measured NMR signal is a current which is generated by the electromotive force (emf) induced in the coil by the precessing magnetization \mathbf{m} and which oscillates with the spin resonance frequency ω_0 . This may be superimposed with another emf due to the external driving, i.e., to the control input (soft pulses regime only). These two oscillating emfs (or, in the AC steady state, the two corresponding oscillating currents, see [Appendix](#) for details) give rise to two magnetic fields. We consider their time-independent components in the rotating frame (taking the rotating wave approximation [5]) and denote them ϕ , for the field due to the spin precession, and \mathbf{u} , for the externally driven field, respectively of components ϕ_x, ϕ_y and u_x, u_y . From (2) and the [Appendix](#), we have that

$$\begin{cases} \phi_x(\mathbf{m}) = \ell \langle \langle \mathbf{m}_0, A_x \mathbf{m} \rangle \rangle = \ell m_y \\ \phi_y(\mathbf{m}) = \ell \langle \langle \mathbf{m}_0, A_y \mathbf{m} \rangle \rangle = -\ell m_x \end{cases} \quad (4)$$

are the field components corresponding to the measured current I_{spin} . Including \mathbf{u} in the model (2), we have

$$\frac{d\mathbf{m}}{dt} = -\delta A_z \mathbf{m} + (u_x + \phi_x(\mathbf{m})) A_x \mathbf{m} + (u_y + \phi_y(\mathbf{m})) A_y \mathbf{m}, \quad (5)$$

for which we have the following obvious result:

Proposition 2. *For the system (5), the norm of the transverse magnetization is constant $\forall t$ if $u_i = -\phi_i(\mathbf{m})$, $i = x, y$.*

In fact, the condition $u_i = -\phi_i(\mathbf{m})$, $i = x, y$ implies that $\dot{\mathbf{m}} = -\delta A_z \mathbf{m}$ which leaves the transverse magnetization invariant.

The electronic feedback suppression of radiation damping of [9], denoted as “Brussels scheme” in [12], works on the current induced by the spin precession in the coil (I_{spin} in the notation of the Appendix) and suppresses it through a suitable circuit. The circuit used in this scheme is designed to create a feedback current proportional to the current flowing in the coil itself. This is done without needing to introduce an additional external field \mathbf{u} (but just using an amplifying circuit as explained in [12]). From (13), suppressing this current (or reducing it by 2–3 orders of magnitude) means suppressing the corresponding field ϕ and hence the radiation damping backaction. This is done in a completely electronic manner, not requiring the use of \mathbf{u} , and it is said in [12] that in the residual (small) current the signal-to-noise ratio is essentially unaltered.

An alternative scheme, called the “École Polytechnique scheme” in [12] works by detecting, inverting and suppressing ϕ through the rf generator and hence through \mathbf{u} , see [10,11] for the original papers. In terms of currents (see Appendix) the scheme can be formulated as $I_{rf}(t) = -I_{spin}(t)$. In our formalism, this corresponds to the feedback of Proposition 2. The exact cancellation of Proposition 2 corresponds to the need for fine-tuning the rf current I_{rf} , specifically its phase and gain as mentioned in [12], and is not a robust operation with respect to any form of uncertainty affecting ϕ . A particular subtask, valid only for the inverted state \mathbf{m}_1 , can however be carried out robustly by means of a high gain feedback law.

Proposition 3. For the system (5), the feedback

$$\begin{aligned} u_x &= -k\phi_x(\mathbf{m}) \\ u_y &= -k\phi_y(\mathbf{m}) \end{aligned} \quad (6)$$

$k > 1$, renders the inverted state \mathbf{m}_1 almost globally asymptotically stable.

Proof. Consider the Lyapunov function of (3) with respect to \mathbf{m}_1 , $V(\mathbf{m}) = \|\mathbf{m}\|^2 - \langle \mathbf{m}_1, \mathbf{m} \rangle$, and differentiate it

$$\begin{aligned} \dot{V}(\mathbf{m}) &= -\langle \mathbf{m}_1, \dot{\mathbf{m}} \rangle \\ &= -(u_x + \phi_x(\mathbf{m}))\langle \mathbf{m}_1, A_x \mathbf{m} \rangle - (u_y + \phi_y(\mathbf{m}))\langle \mathbf{m}_1, A_y \mathbf{m} \rangle \\ &= -(1-k)\phi_x(\mathbf{m})\langle \mathbf{m}_1, A_x \mathbf{m} \rangle - (1-k)\phi_y(\mathbf{m})\langle \mathbf{m}_1, A_y \mathbf{m} \rangle \\ &= (1-k)\ell\langle \mathbf{m}_1, A_x \mathbf{m} \rangle^2 + (1-k)\ell\langle \mathbf{m}_1, A_y \mathbf{m} \rangle^2 \leq 0 \end{aligned}$$

since e.g. $\phi_x(\mathbf{m}) = \langle \mathbf{m}_0, A_x \mathbf{m} \rangle = -\langle \mathbf{m}_1, A_x \mathbf{m} \rangle$. Hence $\dot{V}(\mathbf{m}_1) = 0$ and $\dot{V}(\mathbf{m}) < 0$ for $\mathbf{m} \neq \mathbf{m}_0, \mathbf{m}_1$. The result is valid for any value of ℓ . \square

This use of the “École Polytechnique scheme” for the feedback stabilization of the inverted state is also mentioned in [12]. In terms of the current, it corresponds to inverting and amplifying I_{spin} : $I_{rf} = -kI_{spin}$, $k > 1$. Observe that when $u_x = u_y = 0$, one has $\dot{V} > 0$ i.e., the equilibrium \mathbf{m}_1 indeed becomes unstable, as already mentioned after Proposition 1.

3.1. 2-DOF with feedback stabilization

From the proof of Proposition 3, if $k = 1$ then the closed-loop evolution of the system (5) is only stable but not an attractor ($\dot{V} = 0$ in the proof of Proposition 3) and, from Proposition 2, this corresponds to exact cancellation of the radiation damping. More generally, we may be interested in manipulating the spin state while suppressing at all times the effect of radiation damping. In the “Brussels scheme”, this can be carried out by simply setting $\phi = 0$ in (5), and building a suitable feedback law for \mathbf{u} . In the “École Polytechnique scheme”, we can adopt a 2-degrees of freedom (DOF) control design composed of a prefeedback that cancels the unwanted dynamics linearly superimposed with a

controller that achieves the desired task, e.g. stabilizes the state to the desired orbit of the drift term (i.e., a horizontal circle characterized by a desired value of m_z). The general scheme for such a 2-DOF control design is given by

$$\begin{cases} u_x = -\phi_x(\mathbf{m}) + v_x \\ u_y = -\phi_y(\mathbf{m}) + v_y \end{cases} \quad (7)$$

with v_x, v_y the new control variables. The structure of this 2 DOF controller resembles the one proposed in [13] (similar arguments also appear in [12]), although [13] is not concerned with feedback stabilization. The feedback design of v_x, v_y can for example follow the theory developed in [19]. As in [19], we shall not try to suppress the precession motion (which would introduce singularities in the control law). Rather, we will formulate the stabilization to the orbit given by the desired value of m_z , call it $m_{d,z}$, as a state tracking problem for the dynamical trajectory described by the following system

$$\frac{d\mathbf{m}_d}{dt} = -\delta A_z \mathbf{m}_d. \quad (8)$$

This control technique could be used for example to perform high-precision control as required for NMR quantum information processing—while counteracting the effects of radiation damping, or to improve spectroscopic techniques (for example by actively manipulating the solvent spins while minimizing their radiation damping effects).

The following proposition formalizes this result: a trajectory stabilizing state feedback superimposed with the prefeedback of Proposition 2 achieves asymptotic tracking of $\mathbf{m}_d(t)$.

Proposition 4. Consider the system (5). The 2 DOF feedback controller given by (7) and

$$\begin{cases} v_x = k\langle \mathbf{m}_d, A_x \mathbf{m} \rangle \\ v_y = k\langle \mathbf{m}_d, A_y \mathbf{m} \rangle \end{cases} \quad (9)$$

$k > 0$, tracks the reference trajectory \mathbf{m}_d given by (8) in an asymptotically stable manner for all $\mathbf{m}(0) \in \mathbb{S}^2$ with the exception of the antipodal point $\mathbf{m}(0) = -\mathbf{m}_d(0)$ and of $\mathbf{m}(0), \mathbf{m}_d(0)$ both lying on great horizontal circles.

Proof. Consider the candidate Lyapunov function

$$V = \|\mathbf{m}_d\|^2 - \langle \mathbf{m}_d, \mathbf{m} \rangle$$

and differentiate it:

$$\begin{aligned} \dot{V} &= -\langle \dot{\mathbf{m}}_d, \mathbf{m} \rangle - \langle \mathbf{m}_d, \dot{\mathbf{m}} \rangle \\ &= \delta\langle A_z \mathbf{m}_d, \mathbf{m} \rangle + \delta\langle \mathbf{m}_d, A_z \mathbf{m} \rangle - v_x\langle \mathbf{m}_d, A_x \mathbf{m} \rangle \\ &\quad - v_y\langle \mathbf{m}_d, A_y \mathbf{m} \rangle \\ &= -k(\langle \mathbf{m}_d, A_x \mathbf{m} \rangle^2 + \langle \mathbf{m}_d, A_y \mathbf{m} \rangle^2) \leq 0 \end{aligned}$$

where the cancellation of the two drift terms occurs since $A_z^T = -A_z$. Hence the reference trajectory $\mathbf{m}_d(t)$ is at least stable. The proof of convergence and the analysis of the basin of attraction is now formally identical to that carried out in Proposition 1 of [19] (see also examples in [20]). \square

3.2. Compensating without cancellation through prefeedback

The feedback controller in Proposition 4 requires: (i) full state information (i.e., the on-line knowledge of the Bloch vector \mathbf{m} , retrievable by numerical integration of (5)); (ii) the exact matching of Proposition 2. The interesting question is whether a high gain feedback scheme (similar to Proposition 3) can be obtained without the explicit cancellation of Proposition 2 for the more general task studied in Proposition 4.

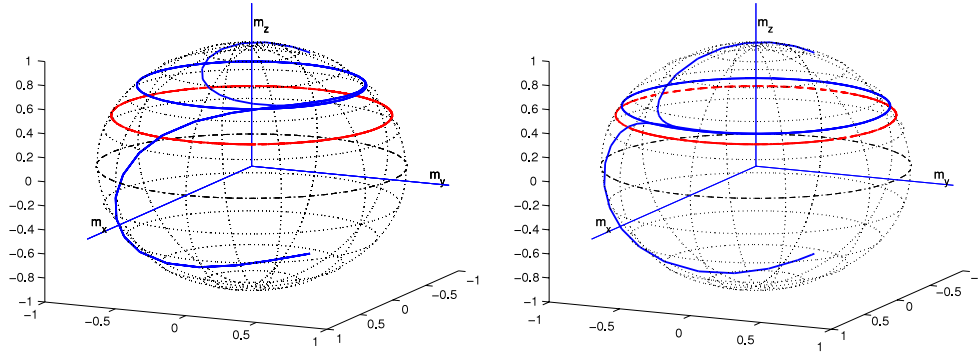


Fig. 1. High gain state feedback stabilization without radiation damping exact compensation. The two plots show each two curves of the system (5) with the feedback (10) from different initial conditions (color online: blue solid lines). Clearly both converge to an orbit that is different from the desired one of (8) (color online: red dashed line). However, in the right plot where a higher gain is used this orbit is closer to the desired one than on the left plot (the ratio of the two gains is 4; the higher value of k is 10 times ℓ).

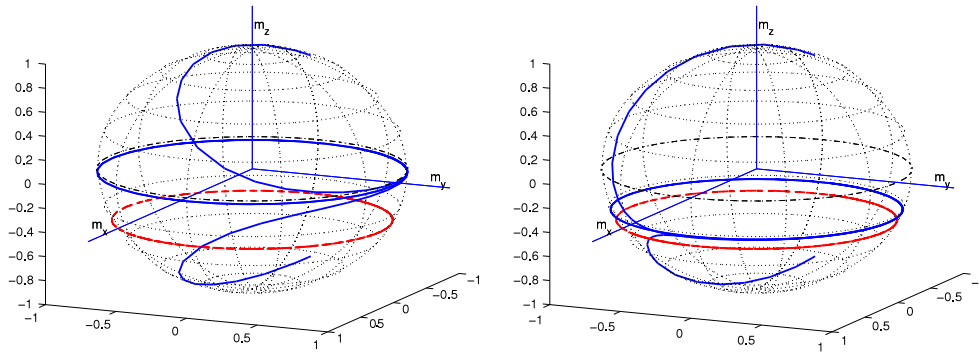


Fig. 2. Steady state tracking error depends on the sign of $m_{d,z}$. The two figures show the same tracking problem as in Fig. 1, with the only difference that now $m_{d,z}$ has negative sign. Proposition 5 predicts that the steady state tracking error is larger than in the case of Fig. 1. This is particularly visible for the low gain situation (left plot).

Proposition 5. Consider the system (5) and the reference trajectory (8). The system with the state feedback

$$\begin{cases} u_x = k\langle \mathbf{m}_d, A_x \mathbf{m} \rangle \\ u_y = k\langle \mathbf{m}_d, A_y \mathbf{m} \rangle \end{cases} \quad (10)$$

$k > 0$, converges to an orbit which approaches the reference trajectory (8) when k is large. The steady state tracking error (i.e., the \mathbb{S}^2 -distance between the two orbits) is $1 - (k + \ell m_{d,z}) / \sqrt{k^2 + \ell^2 + 2k\ell m_{d,z}}$.

Proof. Once again, the argument is based on a Lyapunov function, but for a reference trajectory $\mathbf{M}_f = k\mathbf{m}_d + \ell\mathbf{m}_0$. From (8) $\frac{d\mathbf{M}_f}{dt} = -k\delta A_z \mathbf{m}_d$, but, since $A_z \mathbf{m}_0 = 0$, also $\frac{d\mathbf{M}_f}{dt} = -k\delta A_z \mathbf{M}_f$. Since, typically, $\mathbf{M}_f \notin \mathbb{S}^2$, consider $\mathbf{m}_f = \frac{\mathbf{M}_f}{\|\mathbf{M}_f\|}$, where $\|\mathbf{M}_f\| = \sqrt{k^2 m_{d,x}^2 + k^2 m_{d,y}^2 + (k m_{d,z} + \ell)^2} = \sqrt{k^2 + \ell^2 + 2k\ell m_{d,z}}$. By straightforward calculations, $\frac{d\mathbf{m}_f}{dt} = -\delta A_z \mathbf{m}_f$. This expression implies that considering $V_f = \|\mathbf{m}\|^2 - \langle \mathbf{m}_f, \mathbf{m} \rangle$ and differentiating, the drift terms disappear and we have

$$\begin{aligned} \dot{V}_f &= -\langle \dot{\mathbf{m}}_f, \mathbf{m} \rangle - \langle \mathbf{m}_f, \dot{\mathbf{m}} \rangle \\ &\quad - \langle \mathbf{m}_f, (u_x + \phi_x) A_x \mathbf{m} \rangle - \langle \mathbf{m}_f, (u_y + \phi_y) A_y \mathbf{m} \rangle \\ &= -\langle \mathbf{m}_f, A_x \mathbf{m} \rangle^2 - \langle \mathbf{m}_f, A_y \mathbf{m} \rangle^2 \leq 0 \end{aligned}$$

i.e., we have convergence to $\mathbf{m}_f = (k\mathbf{m}_d + \ell\mathbf{m}_0) / \|\mathbf{M}_f\|$. As $\mathbf{m}_d(t)$ is symmetrically distant from $\mathbf{m}_0 \forall t$, also $\mathbf{m}_f(t)$ is so, meaning that to compute the distance between the attractor orbit \mathbf{m}_f and the desired one \mathbf{m}_d a simple \mathbb{S}^2 -distance can be used, regardless of the initial condition:

$$\begin{aligned} d(\mathbf{m}_f, \mathbf{m}_d) &= 1 - \langle \mathbf{m}_f, \mathbf{m}_d \rangle = 1 - \langle k\mathbf{m}_d + \ell\mathbf{m}_0, \mathbf{m}_d \rangle / \|\mathbf{M}_f\| \\ &= 1 - (k + \ell \langle \mathbf{m}_0, \mathbf{m}_d \rangle) / \|\mathbf{M}_f\| \\ &= 1 - (k + \ell m_{d,z}) / \sqrt{k^2 + \ell^2 + 2k\ell m_{d,z}}. \quad \square \end{aligned}$$

Notice that Proposition 5 still requires full state information, i.e., the numerical evaluation of $\mathbf{m}(t)$. It is clear from Proposition 5 that when the feedback gain k is high (say an order of magnitude higher than ℓ), the steady state tracking error becomes negligible, in particular near the equator. In Fig. 1 we show an example of how this steady state tracking error shrinks when the gain k is increased. Notice how this tracking error depends on the sign of $m_{d,z}$ and is larger for orbits on the lower hemisphere, see Fig. 2.

4. Conclusion

As for many other aspects of the NMR literature, we find that also the methods developed for the purpose of suppressing radiation damping admit nontrivial control theoretical formulations. Part of the aim of this paper is to translate this problem and its solutions into language and techniques familiar to a control audience. In particular, we obtain that feedback control strategies can be classified into two types of methods: high gain feedback and 2 DOF controllers with a prefeedback exactly canceling the radiation damping term. We also show how to use the first type of controller for more general tasks than those considered in the literature, while still not requiring exact knowledge of the radiation damping field (a necessary condition for the methods based on exact cancellation). As for the 2 DOF control design, we show how this can be completed to a true feedback stabilizer that achieves a desired task in an asymptotically stable manner.

Appendix. Model formulation

In this Section we follow essentially [8]. This review paper, which is easily accessible also to an audience with limited knowledge of NMR, provides a more detailed formulation of the model. The collective effect of the ensemble of spins precessing around the z axis is to induce an electromotive force in the receiver coil. In the laboratory frame, according to Faraday's law, this oscillating voltage can be expressed as

$$V_{spin}(t) = -4\pi\xi\eta A \frac{d\mathfrak{M}_x(t)}{dt} \quad (11)$$

where η is the number of turns in the coil, ξ is the filling factor, A is the cross-sectional area of the coil, and \mathfrak{M}_x is the component of the magnetization vector aligned with the laboratory x -axis (conventionally the axis of the coil). Applying Kirchhoff's law to this coil

$$L \frac{d^2 I(t)}{dt^2} + R \frac{dI(t)}{dt} + \frac{I(t)}{C} = \frac{d}{dt} (V_{spin} + V_{rf}) \quad (12)$$

where V_{rf} is the external voltage applied by the generator (i.e., the control input). The natural frequency of the circuit is $\omega = \frac{1}{\sqrt{LC}}$ and its quality factor $Q = \omega L/R$. In the low Q limit, we can assume (following e.g. [18]), that the damping part of this damped harmonic oscillator is quickly exhausted, and work at the resulting AC steady state, assuming that also the external signal V_{rf} is a soft pulse (i.e., slowly varying in the rotating frame). This leads to $V_{spin} + V_{rf} = ZI(t)$, where the impedance Z is a function of ω , ω_0 , Q , and L [18]. Special devices, such as the directional coupler circuit described in [12], allow to distinguish in $I(t)$ the two components due to the spin precession and to the external generator: $I(t) = I_{spin}(t) + I_{rf}(t)$. Each oscillating current induces a field. In the frame rotating with the circuit frequency ω , the two fields are denoted \mathbf{u} and ϕ . For example,

$$I_{spin}(t) = \sqrt{\frac{\text{Vol}}{\pi L}} |\phi| \cos(\omega t + \psi) \quad (13)$$

where Vol is the coil volume and ψ is the phase of the current. As the components of \mathbf{m} are related to \mathfrak{M}_x by

$$\mathfrak{M}_x = M_0 [m_x \cos(\omega t) \mathbf{e}_x + m_y \sin(\omega t) \mathbf{e}_y], \quad (14)$$

by inserting Eqs. (11) and (13) into (12), we obtain the components of the field ϕ as used in (4) in the limit of low Q and of the slowly varying modulus approximation [8,21].

References

- [1] A. Abragam, Principles of Nuclear Magnetism, Oxford Univ. Press, 1961.
- [2] C.P. Slichter, Principles of Magnetic Resonance, 3rd ed., Springer-Verlag, 1996.
- [3] R. Ernst, G. Bodenhausen, A. Wokaun, Principles of Nuclear Magnetic Resonance in One and Two Dimensions, Clarendon Press, Oxford, 1987.
- [4] M.H. Levitt, Prog. Nucl. Magn. Reson. Spectrosc. 18 (61) (1986).
- [5] U. Haeberlen, High Resolution NMR in Solids: Selective Averaging, Academic Press Inc., 1976.
- [6] N. Bloembergen, R.V. Pound, Radiation damping in magnetic resonance experiments, Phys. Rev. 95 (1) (1954) 8–12.
- [7] S. Bloom, Effects of radiation damping on spin dynamics, J. Appl. Phys. 28 (7) (1957) 800–805.
- [8] M. Augustine, Transient properties of radiation damping, Prog. Nucl. Magn. Reson. Spectrosc. 40 (2) (2002) 111–150.
- [9] P. Broekaert, J. Jeener, Suppression of radiation damping in NMR in liquids by active electronic feedback, J. Magn. Reson. 113 (1) (1995) 60–64.
- [10] A. Louis-Joseph, D. Abergel, J.-Y. Lallemand, Neutralization of radiation damping by selective feedback on a 400 MHz NMR spectrometer, J. Biomolecular NMR 99 (1995).
- [11] D. Abergel, C. Carlotti, A. Louis-Joseph, J.-Y. Lallemand, Improvements in radiation-damping control in high-resolution NMR, J. Magn. Reson. B 109 (2) (1995) 218–222.
- [12] J. Jeener, Collective effects in liquid NMR: dipolar field and radiation damping, Encyc. Nucl. Magn. Reson. 9 (2002) 642–679.
- [13] J. Chen, B. Cutting, G. Bodenhausen, Measurement of radiation damping rate constants in nuclear magnetic resonance by inversion recovery and automated compensation of selective pulses, J. Chem. Phys. 112 (15) (2000) 6511–6514.
- [14] D. Abergel, Chaotic solutions of the feedback driven Bloch equations, Phys. Lett. A 302 (2002) 17–22.
- [15] D. Abergel, A. Louis-Joseph, J. Lallemand, Self-sustained maser oscillations of a large magnetization driven by a radiation damping-based electronic feedback, J. Chem. Phys. 116 (16) (2002) 7073–7080.
- [16] M. Augustine, S. Bush, E. Hahn, Noise triggering of radiation damping from the inverted state, Chem. Phys. Lett. 322 (1–2) (2000) 111–118.
- [17] A. Sodickson, W.E. Maas, D.G. Cory, The initiation of radiation damping by noise, J. Magn. Reson. B 110 (1996) 298–303.
- [18] A. Vlassenbroek, J. Jeener, P. Broekaert, Radiation damping in high resolution liquid NMR: a simulation study, J. Chem. Phys. 103 (14) (1995) 5886–5897.
- [19] C. Altafini, Feedback control of spin systems, Quantum Inf. Process. 6 (2007) 9–36.
- [20] C. Altafini, Feedback stabilization of isospectral control systems on complex flag manifolds: application to quantum ensembles, IEEE Trans. Autom. Control 52 (11) (2007) 2019–2028.
- [21] M.P. Augustine, E.L. Hahn, Three-component spin echoes, J. Phys. Chem. B 102 (42) (1998) 8229–8238.