

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

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In NMR spectroscopy, the collective measurement 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 this radiation damping. It is shown that the two feedback schemes commonly used in the NMR practice correspond one to a high gain output feedback for the simple case of maintaining the spin $1/2$ in its inverted state, and the second to a 2-degree of freedom control design with a prefeedback that exactly cancels the radiation damping field. A general high gain feedback stabilization design not requiring the knowledge of the radiation damping time constant is also investigated.

I. INTRODUCTION

In recent years, the theory [11, 13, 16, 18, 19] and practice [14] of (real-time) feedback for quantum mechanical systems has gained momentum especially in contexts such as quantum optics [19]. In order to avoid wavefunction collapse, the measurement is assumed weak and the feedback is seen as a way to influence the resulting dynamics conditioned by the measurement back-action. This conditioning is stochastic for a single isolated quantum system [18], but can assume the form of a deterministic back-action when considering the expectation values for an ensemble of systems [12, 16, 17]. In this last setting, the effect of a weak measurement is described by a term in a Markovian master equation which can be conservative (when the measurement is perfect, i.e., lossless) or dissipative (imperfect measurement).

In NMR spectroscopy, in presence of a collective spin measurement the phenomenon occurring is called radiation damping [5, 7, 8], and it is due to the electromagnetic field induced by the current passing through the detection coil while doing a measurement. This field in turn interacts with the spins in the sample, hence it induces a back-action on the system observed. If back-actions are hallmarks of quantum measurement, magnetic resonance is no exception in this respect.

In high field and probes of high quality factor, radiation damping is typically an important effect at certain frequency ranges, for example that of the abundant spin of the solvent. For these, it behaves much like a soft pulse steering the magnetization vector back to its equilibrium value. For other bandwidths, the back-action signal is so weak it is dominated by the relaxation effects, and hence it is negligible. In this work we assume to be dealing with one of those situations in which radiation damping is of interest and relaxation is negligible.

An accepted model of radiation damping exists only for the spin $1/2$ case, and its formulation closely resembles the back-action term mentioned above for generic quantum systems under weak measurements, only it is always assumed to be conservative, i.e., to preserve the norm of the Bloch vector. The efforts to engineer the NMR receiving/transmitting system in order to reject this form of back-action have a longer history than in other quantum systems and by now there are many ways to compensate for it, such as electronic feedback [9], rf pulse compensation [10], gradient field, or composite pulse sequences. We are here interested only in the first two methods, which are standard in high-resolution NMR spectrometers.

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 [1, 2, 5, 6, 15]. Second, we aim to give a

system-theoretic interpretation of the electronic feedback and pulse compensation control designs. We will show that the first scheme can be thought of as a high gain output regulation controller in which the lateral magnetization is the output of the system. In this case, the basic task studied in [9], namely canceling the current in the only coil that works both as a receiver and as an actuator, means regulating the output to zero, and corresponds to trying to maintain the spin 1/2 in the “fully inverted” state (south pole of the Bloch sphere), although it works only for this particular state. As for the second scheme [10], it can be thought of as a prefeedback that cancels exactly the radiation damping dynamics and which can be superimposed to another active field (on the same coil) in order to generate desired control actions via soft, as well as hard, pulses. In control terms, this design is a 2-degrees of freedom (DOF) control design.

The third and last aim of this paper is to explore possible alternative schemes inspired by control theory. We will see that 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 cancelation, this feedback controller does not require the explicit knowledge of the radiation damping time constant. For “high gain” we mean a ratio of around an order of magnitude between the signal produced in the coil to transmit the actuation command and the NMR signal corresponding to (unactuated, i.e., “passive”) measurement. Hence this task of radiation damping compensation can be performed in the soft pulse regime and therefore, in principle, measurement and actuation can be performed simultaneously on the same coil. In turn this implies that real-time feedback makes sense in this context even with a single coil available. When strong pulses are instead considered, the above 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.

II. THE MODEL FOR RADIATION DAMPING

In the following, we shall focus only on the spin 1/2 case, the only one for which an accepted model of radiation damping exists [5, 7, 8]. Disregarding relaxation effects (i.e., in the limit $T_1 = T_2 = \infty$) and denoting with $\mathbf{m} = [m_x \ m_y \ m_z]^T$ the normalized Bloch vector, ($\mathbf{m} = \mathbf{M}/M_o$ where M_o is the equilibrium magnetization), the nonlinear Bloch equations for radiation damping in a frame rotating with the circuit resonant frequency are

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

where $\delta = \omega - \omega_o$ is the offset between the Larmor precession frequency ω_o and the circuit resonant frequency ω , ℓ is the radiation damping rate $\ell = \frac{1}{\gamma T_R}$, with γ the gyromagnetic ratio and T_R the radiation damping time constant $T_R = \frac{1}{2\pi\xi M_o Q}$ (ξ = coil filling factor, Q = probe quality factor) [2, 5, 8]. Denoting A_x , A_y and A_z the real rotation matrices around the x , y , and z axis, $\text{Lie}(A_x, A_y, A_z) = \text{span}(A_x, A_y, A_z) = \mathfrak{so}(3)$, then (1) can be written as

$$\frac{d\mathbf{m}}{dt} = -\delta A_z \mathbf{m} + \ell \langle \mathbf{m}_o, A_x \mathbf{m} \rangle A_x \mathbf{m} + \ell \langle \mathbf{m}_o, A_y \mathbf{m} \rangle A_y \mathbf{m}\tag{2}$$

where $\mathbf{m}_o = [001]^T$ is the north pole of the Bloch sphere (aligned with the static magnetic field applied to the ensemble) and $\langle \cdot, \cdot \rangle$ denotes an Euclidean inner product in \mathbb{R}^3 .

Proposition 1 *The system (2) has \mathbf{m}_o as an almost globally asymptotically stable equilibrium point, with region of attraction $\mathbb{S}^2 \setminus \{\mathbf{m}_1\}$, where $\mathbf{m}_1 = [00-1]^T$ is the south pole of the Bloch sphere.*

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

$$V = \|\mathbf{m}\| - \langle \mathbf{m}_o, \mathbf{m} \rangle.$$

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

$$\dot{V} = -\langle \mathbf{m}_o, \dot{\mathbf{m}} \rangle = \delta \langle \mathbf{m}_o, A_z \mathbf{m} \rangle - \ell \langle \mathbf{m}_o, A_x \mathbf{m} \rangle \langle \mathbf{m}_o, A_x \mathbf{m} \rangle - \ell \langle \mathbf{m}_o, A_y \mathbf{m} \rangle \langle \mathbf{m}_o, A_y \mathbf{m} \rangle$$

Since $A_z \mathbf{m}_o = [000]^T$, the first term disappears and hence

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

Hence $V(\cdot)$ is a Lyapunov function for the equilibrium \mathbf{m}_o of (2). As $\dot{V} = 0$ only for $\mathbf{m} = \mathbf{m}_o$ or $\mathbf{m} = \mathbf{m}_1$, \mathbf{m}_o 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}_o [6, 15].

III. FEEDBACK CONTROL STRATEGIES

The electronic feedback suppression of radiation damping of [9] works on the current obtained from the measurement coil and compensates for it inducing a field on the spins through the same coil.

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 induced in the coil by the magnetic field and which oscillates with the circuit resonance frequency ω . However, for all practical purposes we can assume to be measuring directly the two components of the lateral magnetization $i_x(t) = \eta m_x$, $i_y = \eta m_y$, where η is an efficiency factor. Clearly $\sqrt{m_x^2 + m_y^2} \leq 1$ with equal sign reached only at the equator. Since $\|\mathbf{m}\| = 1$, the norm of the output vector $i_c(t) = \eta \sqrt{m_x^2 + m_y^2} = \eta \sqrt{1 - m_z^2}$ is the amplitude of the current measured by the apparatus. If we consider i_x, i_y as outputs of the system and include the control terms u_x, u_y for the rf fields (on the same coil as the measurement but externally driven) then (2) becomes:

$$\begin{aligned} \frac{d\mathbf{m}}{dt} &= -\delta A_z \mathbf{m} + (u_x + \phi_x(\mathbf{m})) A_x \mathbf{m} + (u_y + \phi_y(\mathbf{m})) A_y \mathbf{m} \\ \begin{bmatrix} i_x \\ i_y \end{bmatrix} &= \eta \begin{bmatrix} m_x \\ m_y \end{bmatrix} \end{aligned} \quad (3)$$

where

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

Remark 1 Since the system (3) is conservative, the bidimensional output in (3) allows to recover the entire Bloch vector $\mathbf{m} \in \mathbb{S}^2$ up to the sign of m_z . Hence our distinction between “state” and “output” feedback design reduces in practice to the knowledge of $\text{sign}(m_z)$.

In practice, since any NMR experiment entails a preparation of the “true” initial state $\mathbf{m}(0)$, $m_z(t)$ can be reconstructed by numerical integration.

Proposition 2 The output of (3) has constant norm $i_c(t) \forall t$ if and only if $u_i = -\phi_i(\mathbf{m})$, $i = x, y$.

Proof. The condition $u_i = -\phi_i(\mathbf{m})$, $i = x, y$ implies that $\dot{\mathbf{m}} = -\delta A_z \mathbf{m}$ which leaves the lateral magnetization and hence i_c invariant. For the other direction, $m_x^2 + m_y^2 = 1 - m_z^2 = \text{const} \forall t$ implies that $\dot{m}_z = 0$. From (1) and (2), this yields

$$\ell(m_x^2 + m_y^2) + u_x m_y - u_y m_x = 0$$

i.e.,

$$(\ell m_x - u_y) m_x + (\ell m_y + u_x) m_y = 0 \quad \forall m_x, m_y \text{ such that } m_x^2 + m_y^2 = \text{const.}$$

This is obviously satisfied only when $\ell m_x - u_y = 0$ and $\ell m_y + u_x = 0$ simultaneously. \square

In [9], the electronic feedback scheme is based on considering the output current as a signal to reject i.e., the feedback task is formulated as $i_c(t) \rightarrow 0$. Clearly, from Proposition 2, $i_c(t) = 0$ if and only if $m_x^2 + m_y^2 = 0$ i.e., on $\mathbf{m} = \{\mathbf{m}_o, \mathbf{m}_1\}$, meaning that in practice it works to reject radiation damping only for the inverted state.

Suppressing the output current through a negative feedback circuit entails the suppression of the radiation damping. In fact, in absence of external driving, if the back-action due to radiation damping induces a current i_c and a field of components $\phi_x(\mathbf{m})$, $\phi_y(\mathbf{m})$, suppressing that current then means suppressing the radiation damping field. Hence the output regulation result of [9] can be formalized for our model as follows.

Proposition 3 For the system (3), the output feedback

$$\begin{aligned} u_x &= -k\phi_x(\mathbf{m}) \\ u_y &= -k\phi_y(\mathbf{m}) \end{aligned} \quad (5)$$

$k > 1$, renders the south pole \mathbf{m}_1 asymptotically stable on the open lower emisphere $\mathbb{E}_1 = \{\mathbf{m} \in \mathbb{S}^2 \text{ s. t. } m_z < 0\}$.

Proof. It follows from (4) that the feedback design (5) is indeed an output feedback (no knowledge of m_z is required). Consider the function $W = i_c^2 \geq 0 \forall \mathbf{m} \in \mathbb{S}^2$, $W = 0$ only in $\mathbf{m}_o, \mathbf{m}_1$. Its derivative is

$$\begin{aligned} \frac{dW}{dt} &= 2\eta^2(m_x\dot{m}_x + m_y\dot{m}_y) = 2\eta^2(-\ell m_z(m_x^2 + m_y^2) + u_y m_x m_z - u_x m_y m_z) \\ &= -2\ell m_z i_c^2 + 2\eta^2 m_z (u_y m_x - u_x m_y) \end{aligned} \quad (6)$$

Inserting the feedback (5),

$$\frac{dW}{dt} = -2\ell m_z i_c^2 + 2\eta^2 \ell k m_z (m_x^2 + m_y^2) = 2\ell m_z i_c^2 (-1 + k) < 0 \quad \forall \mathbf{m} \in \mathbb{E}_1 \setminus \{\mathbf{m}_1\}$$

□

Observe in the last row of (6) that when $u_x = u_y = 0$, since $m_z < 0$ near \mathbf{m}_1 , one has $\dot{W} > 0$ i.e., the equilibrium \mathbf{m}_1 becomes unstable, as already shown in Proposition 1.

Remark 2 While the exact cancellation of Proposition 2 requires the knowledge of ℓ (and hence of the radiation damping time constant T_R), the feedback (5) works for any ℓ (for sufficiently high gain k).

From the proof of Proposition 3, if $k = 1$ then the evolution is only stable but not an attractor ($\dot{W} = 0$ in absence of external controls) and, from Proposition 2, this corresponds to exact cancelation of the radiation damping.

In the case of Proposition 3, the task is to regulate the output to 0. More generally, we may be interested in manipulating the spin state while suppressing at all times the effect of radiation damping. For this scope, we can adopt a 2-degrees of freedom (DOF) control design composed of a prefeedback that cancels the unwanted dynamics plus a controller that achieves the desired task, e.g. stabilize 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 output 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. This 2 DOF controller is the one proposed in [10]. The design of v_x, v_y can for example follow the theory developed in [3]. As in [3], 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

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

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

Proposition 4 Consider the system (3). The 2 DOF state 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:

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

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 [3] (see also examples in [4]). \square

IV. COMPENSATING WITHOUT KNOWLEDGE OF ℓ

The feedback controller in Proposition 4 requires: i) full state information (i.e., the knowledge of m_z , especially its sign, which is not directly retrievable from the output equation); ii) the knowledge of ℓ (i.e., of the time constant T_R of the radiation damping). The interesting question is whether a high gain (state or output) feedback scheme (similar to Proposition 3) can be obtained without the explicit knowledge of ℓ for the more general task studied in Proposition 4.

Proposition 5 Consider the system (3) and the reference trajectory (8). Assuming that the radiation damping rate ℓ is unknown, 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 $\mathbf{M}_f = k\mathbf{m}_d + \ell\mathbf{m}_o$. From (8) $\frac{d\mathbf{M}_f}{dt} = -k\delta A_z \mathbf{m}_d$, but, since $A_z \mathbf{m}_o = 0$, 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 $\|\mathbf{M}_f\| = \sqrt{k^2 m_{d,x}^2 + k^2 m_{d,y}^2 + (k m_{d,z} + \ell)^2} = \sqrt{k^2 + \ell^2 + 2k\ell m_{d,z}}$, and, consequently, $\frac{d\mathbf{m}_f}{dt} = -\delta A_z \mathbf{m}_f$. 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 $\mathbf{m}_f = (k\mathbf{m}_d + \ell\mathbf{m}_o) / \|\mathbf{M}_f\|$. As $\mathbf{m}_d(t)$ is symmetrically distant from $\mathbf{m}_o \forall t$, 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:

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

\square

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.

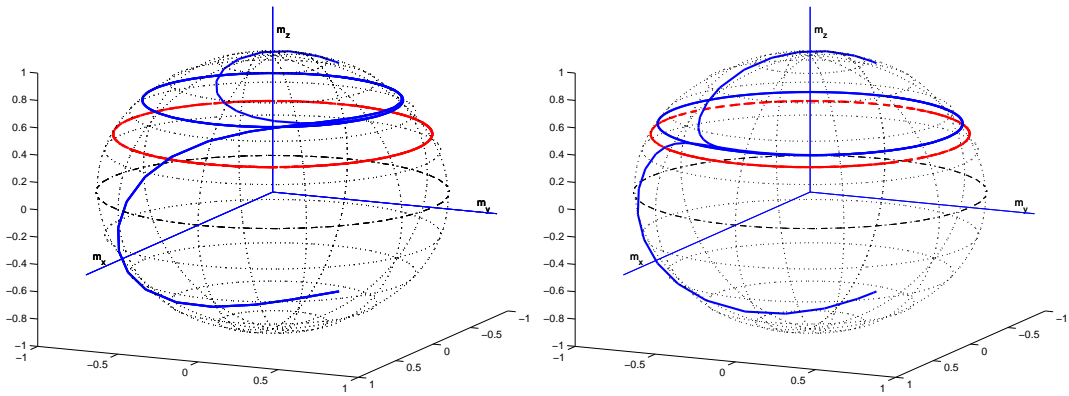


FIG. 1: High gain state feedback stabilization without radiation damping exact compensation. The two plots show each two curves of the system (3) with the feedback (10) from different initial conditions (blue solid lines). Clearly both converge to a orbit that is different from the desired one of (8) (shown in 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).

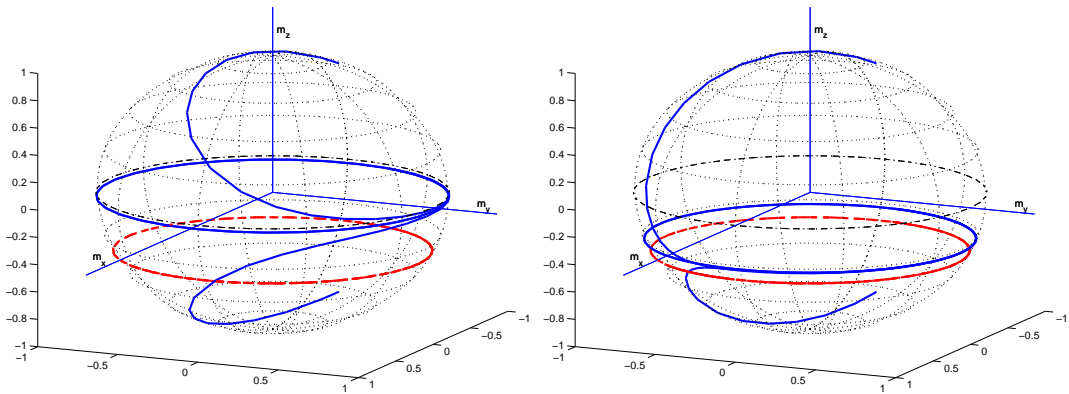


FIG. 2: Steady state tracking error depends on the sign of $m_{d,z}$. The two figures show the same tracking problem as in Fig. 1, with the only difference that now $m_{d,z}$ has negative sign. Proposition 5 predicts that the steady state tracking error is larger than in the case of Fig. 1. This is particularly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

V. CONCLUSION

As for many other aspects of the NMR literature, we find that also the methods developed for the purpose of suppressing radiation damping admitt 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 considered in the literature, while still not requiring exact knowledge of the time constant of radiation damping (a necessary condition for the methods based on exact cancellation).

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