Systems & Control Letters 113 (2018) 36–44

Contents lists available at ScienceDirect

Systems & Control Letters

journal homepage: www.elsevier.com/locate/sysconle

Asymptotic ensemble stabilizability of the Bloch equation

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ARTICLE INFO

Article history:
Received 9 April 2017
Received in revised form 4 January 2018
Accepted 16 January 2018
Available online 2 February 2018

Keywords:
Ensemble controllability
Quantum control

ABSTRACT

In this paper we are concerned with the stabilizability at an equilibrium point of an ensemble of non interacting half-spins. We assume that the spins are immersed in a static magnetic field, with dispersion in the Larmor frequency, and are controlled by a time varying transverse field. Our goal is to steer the whole ensemble to the uniform "down" position.

Two cases are addressed: for a finite ensemble of spins, we provide a control function (in feedback form) that asymptotically stabilizes the ensemble to the "down" position, generically with respect to the initial condition. For an ensemble containing a countable number of spins, we construct a sequence of control functions such that the sequence of the corresponding solutions pointwise converges, asymptotically in time, to the target state, generically with respect to the initial conditions.

The control functions proposed are uniformly bounded and continuous.

1. Introduction

Ensemble controllability (also called *simultaneous controllability*) is a notion introduced in [1–3] for quantum systems described by a family of parameter-dependent ordinary differential equations; it concerns the possibility of finding control functions that compensate the dispersion in the parameters and drive the whole family (ensemble) from some initial state to some prescribed target state.

Such an issue is motivated by recent engineering applications, such as, for instance, quantum control (see for instance [3–6] and references therein), distributed parameters systems and PDEs [7–11], and flocks of identical systems [12].

General results for the ensemble controllability of linear and nonlinear systems, in continuous and discrete time, can be found in the recent papers [13–17].

This paper deals with the simultaneous control of an ensemble of half-spins immersed on a magnetic field, where each spin is described by a magnetization vector $\boldsymbol{M} \in \mathbb{R}^3$, subject to the dynamics $\frac{d\boldsymbol{M}}{dt} = -\gamma \boldsymbol{M} \times \boldsymbol{B}(\boldsymbol{r}, t)$, where $\boldsymbol{B}(\boldsymbol{r}, t)$ is a magnetic field composed by a static component directed along the z-axis, and a time varying component on the xy-plane, called *radio-frequency (rf) field*, and γ denotes the gyromagnetic ratios of the spins. In this system, since all spins are controlled by the same magnetic field $\boldsymbol{B}(\boldsymbol{r}, t)$, the spatial dispersion in the amplitude of the magnetic field gives rise to the following inhomogeneities in the dynamics: *rf inhomogeneity*, caused by dispersion in the radio-frequency field, and a spread in the Larmor frequency, given by dispersion of the static component of the field. This problem arises, for instance, in NMR spectroscopy (see [18] and references in [19,3,4]).

The task of controlling such system is wide, multi-faceted and very rich, depending on the cardinality of the set of the spin to be controlled (and the topology of this set), on the particular notion of controllability addressed, and on the functional space where control functions live.

The above-cited articles [1–3] are concerned with both rf inhomogeneity and Larmor dispersion, with dispersion parameters that belong to some compact domain $\mathcal{D}$. The magnetization vector of the system is thus a function on $\mathcal{D}$, taking values in the unit sphere of $\mathbb{R}^3$, and ensemble controllability has to be intended as convergence in the $L^\infty(\mathcal{D}, \mathbb{R}^3)$-norm. The controllability result is achieved by means of Lie algebraic techniques coupled with adiabatic evolution, and holds for both bounded and unbounded controls.

In [4], the authors focus on systems subject to Larmor dispersions, and provide a complete analysis of controllability properties of the ensemble in different scenarios, such as: bounded/unbounded controls; finite time/asymptotic controllability; approximate/exact controllability in the $L^2(\mathcal{D}, \mathbb{R}^3)$ norm; boundedness/unboundedness of the set $\mathcal{D}$. In particular, results on exact local controllability with unbounded controls are provided.

In this paper we consider an ensemble of Bloch equations presenting Larmor dispersion, with frequencies belonging to some bounded subset $\mathcal{E} \subset \mathbb{R}$. Coupling a Lyapunov function approach with some tools of dynamical systems theory, we exhibit a control function (in feedback form) that approximately drives, asymptotically in time and generically with respect to the initial conditions,

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https://doi.org/10.1016/j.sysconle.2018.01.008
0167-6911/

all spins to the "down" position. Two cases are addressed: if the set $\mathcal{E}$ is finite, our strategy provides exact exponential stabilizability in infinite time, while in the case where $\mathcal{E}$ is a countable collection of energies, our approach implies asymptotic pointwise convergence towards the target state.

Feedback control is a widely used tool for stabilization of control-affine systems (see for instance [20,21] and references therein).

Concerning the stabilization of ensembles, we mention two papers using this approach: in [19], the author aims at stabilizing an ensemble of interacting spins along a reference trajectory; the result is achieved by showing, by means of Lie-algebraic methods, that the distance between the state of the system and the target trajectory is a Lyapunov function. In [22], Jurdjevic–Quinn conditions are applied to stabilize an ensemble of harmonic oscillators.

The feedback form of the control guarantees more robustness with respect to open-loop controls, and gives rise to a continuous bounded control, more easy to implement in practical situations. We stress that, in the finite dimensional case, the implementation of the control requires the knowledge of the *bulk magnetization* of all spins, which is accessible through classical measurements (see for instance [23,19]). We finally remark that the control proposed in this paper is very similar to the *radiation damping effect* arising in NMR (see [24,25]); we comment this fact in the conclusion.

The structure of the paper is the following: in Section 2 we state the problem in general form; in Section 3 we tackle the finite dimensional case, while in Section 4 we analyze the case of a countable family of systems. Section 5 is devoted to some numerical results.

2. Statement of the problem

We consider an ensemble of non-interacting spins immersed in a static magnetic field of strength $B_0(\boldsymbol{r})$, directed along the z-axis, and a time varying transverse field $(B_x(t), B_y(t), 0)$ (rf field), that we can control. The Bloch equation for this system takes then the form

$$\frac{\partial \boldsymbol{M}}{\partial t}(\boldsymbol{r}, t) = \begin{pmatrix} 0 & -B_0(\boldsymbol{r}) & B_y(t) \\ B_0(\boldsymbol{r}) & 0 & -B_x(t) \\ -B_y(t) & B_x(t) & 0 \end{pmatrix} \boldsymbol{M}((\boldsymbol{r}), t) \tag{1}$$

(here for simplicity we set $\gamma = 1$). For more details, we mention the monograph [26].

Since the dependence on the spatial coordinate $\boldsymbol{r}$ appears only in $B_0(\boldsymbol{r})$, we can represent $M(\boldsymbol{r}, t)$ as a collection of time-dependent vectors $X_e(t) = (x_e(t), y_e(t), z_e(t))$, where $e = B_0(\boldsymbol{r})$, each one belonging to the unit sphere $S^2 \subset \mathbb{R}^3$ and subject to the law

$$\begin{pmatrix} \dot{x}_e \\ \dot{y}_e \\ \dot{z}_e \end{pmatrix} = \begin{pmatrix} 0 & -e & u_2 \\ e & 0 & u_1 \\ -u_2 & -u_1 & 0 \end{pmatrix} \begin{pmatrix} x_e \\ y_e \\ z_e \end{pmatrix}, \tag{2}$$

with $u_1(t) = -B_x(t)$ and $u_2(t) = B_y(t)$. The Larmor frequencies e of the spins in the ensemble take value in some subset $\mathcal{E} \subset I$ of a bounded interval I. Depending on the spatial distribution of the spins, $\mathcal{E}$ could be a finite set, an infinite countable set, or an interval.

We are concerned with the following control problem:

(P) *Design a control function* $\mathbf{u} : [0, +\infty) \to \mathbb{R}^2$ *such that for every* $e \in \mathcal{E}$ *the solution of* Eq. (2) *is driven to* $X_e = (0, 0, -1)$.

To face this problem, we consider the Cartesian product $\boldsymbol{S} = \prod_{e\in\mathcal{E}} S^2$, whose elements are the collections $\boldsymbol{X} = \{X_e\}_{e\in\mathcal{E}}$ such that $X_e \in S^2$ for every $e \in \mathcal{E}$. Depending on the structure of $\mathcal{E}$, $\boldsymbol{X}$ can be a finite or an infinite countable collection of states $X_e \in S^2$, or a function $\boldsymbol{X} : \mathcal{E} \to S^2$ belonging to some functional space. The collection $\boldsymbol{X}$ of magnetic moments evolves according to the equation

$$\dot{\Xi} = \boldsymbol{F}(\Xi, \mathbf{u}), \qquad \Xi(0) = \boldsymbol{X}, \tag{3}$$

where $\boldsymbol{F}$ denotes the collection $\boldsymbol{F} = \{F_e\}_{e\in\mathcal{E}}$ of tangent vectors to S^2, with $F_e(\boldsymbol{X}, \mathbf{u}) = \begin{pmatrix} 0 & -e & u_2 \\ e & 0 & u_1 \\ -u_2 & -u_1 & 0 \end{pmatrix} X_e$, and $\mathbf{u} = (u_1, u_2)$.

Some remarks on the existence of solutions for Eq. (3) are in order, and will be provided case by case. Assuming that these issues are already fixed, we define the two states $\boldsymbol{X}^+ = \{X_e : \forall e \in \mathcal{E}\; X_e = (0, 0, 1)\}$ and $\boldsymbol{X}^- = \{X_e : \forall e \in \mathcal{E}\; X_e = (0, 0, -1)\}$, and rewrite the problem **(P)** as

(P′) *Design a control function* $\mathbf{u} : [0, +\infty) \to \mathbb{R}^2$ *such that the solution of* Eq. (3) *is driven to* $\boldsymbol{X} = \boldsymbol{X}^-$.

We remark that the notion of convergence of $\boldsymbol{X}(\cdot)$ towards $\boldsymbol{X}^-$ in problem (**P′**) has to be specified case by case, depending on the structure of the set $\mathcal{E}$ and on the topology of $\boldsymbol{S}$.

3. Finite dimensional case

First of all, we consider the case in which the set $\mathcal{E}$ is a finite collection of pairwise distinct energies, that is $\mathcal{E} = (e_1, \ldots, e_p)$ such that $e_k \in I\; \forall k \in \{1, \ldots, p\}$ and $e_k \neq e_j$ if $i \neq j$. We recall that the state space $\boldsymbol{S}$ of the system is the finite product of p copies of S^2.

Lemma 1. *Assume that all energy levels e_i are pairwise distinct. Let $\mathcal{I} = \{\boldsymbol{X} \in \boldsymbol{S} : x_{e_i} = y_{e_i} = 0\; \forall\, i = 1, \ldots, p\}$. Then every solution of the control system* (2) *with control*

$$\begin{cases} u_1 = \sum_{i=1}^{p} y_{e_i} \\ u_2 = \sum_{i=1}^{p} x_{e_i} \end{cases} \tag{4}$$

tends to $\mathcal{I}$ as $t \to +\infty$.

Proof. Consider the function $V(\boldsymbol{X}) = \sum_{i=1}^{p} z_{e_i}$, and let $\Xi(\cdot)$ be a solution of (3) with the control given in (4). We notice that $\dot{V}(\Xi(t)) = -\left(\sum_{i=1}^{p} x_{e_i}\right)^2 - \left(\sum_{i=1}^{p} y_{e_i}\right)^2$, therefore it is non-positive on the whole $\boldsymbol{S}$, and it is zero only on the set $\mathcal{M} = \{\boldsymbol{X} \in \boldsymbol{S} : \sum_{i=1}^{p} x_{e_i} = \sum_{i=1}^{p} y_{e_i} = 0\}$. We can then apply La Salle invariance principle to conclude that, for every initial condition, $\Xi(t)$ tends to the largest invariant subset of $\mathcal{M}$.

Consider a trajectory $\Xi(\cdot)$ entirely contained in $\mathcal{M}$. Since $\mathbf{u} = 0$, then for every i we have that

$$\Xi_i(t) = \begin{pmatrix} \cos(e_i t) & -\sin(e_i t) & 0 \\ \sin(e_i t) & \cos(e_i t) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_{e_i}(0) \\ y_{e_i}(0) \\ z_{e_i}(0) \end{pmatrix}.$$

By definition, for every $t \geq 0$ it holds $\sum_{i=1}^{p} x_{e_i}(t) = \sum_{i=1}^{p} y_{e_i}(t) = 0$. Differentiating these equalities $p-1$ times and evaluating at $t = 0$ we obtain the two conditions

$$\begin{pmatrix} 1 & 1 & \ldots & 1 \\ e_1 & e_2 & \ldots & e_p \\ \vdots & \vdots & & \\ e_1^{p-1} & e_2^{p-1} & \ldots & e_p^{p-1} \end{pmatrix} \begin{pmatrix} x_1(0) \\ x_2(0) \\ \vdots \\ x_p(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 & \ldots & 1 \\ e_1 & e_2 & \ldots & e_p \\ \vdots & \vdots & & \\ e_1^{p-1} & e_2^{p-1} & \ldots & e_p^{p-1} \end{pmatrix} \begin{pmatrix} y_1(0) \\ y_2(0) \\ \vdots \\ y_p(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$