FFC NMR Relaxometers on Education

Topologies, control techniques and electromagnetic devices

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***Abstract*—The Fast Field Cycling (FFC) Nuclear Magnetic Resonance (NMR) equipment has been mainly developed by engineers with a strong background in power electronics, control and physics. This technique has been widely used by physicists, chemists, biologists, pharmacists and food analysts. During the last decades, the development of this type of apparatus has been taking advantage of the power semiconductors, topologies of the power electronic converters, control techniques, computational tools and materials, among other aspects. In this paper, teaching aspects of using this type of equipment and technique in courses of physics and electrical engineering is described.**

***Keywords*—power electronics; control; semiconductors; experiment; computational tools**

I. Introduction

Fast Field Cycling (FFC) Nuclear Magnetic Resonance (NMR) is an experimental and powerful technique used to study the molecular dynamics of different types of compounds [1-4]. The main modules of a FFC NMR apparatus, represented in Fig. 1, are:

- Power supply/Current source;
- Magnet;
- Control;
- Radio frequency system;
- Computer/Software;
- Temperature controller.

During the last decades, different solutions for each module have been developed. If during the early days of the technique this equipment was operated manually and was constituted by mechanical parts, the most recent solutions incorporate advanced electronic circuits and can also be digitally controlled. Furthermore, efficient and portable solutions have been developed [5-8].

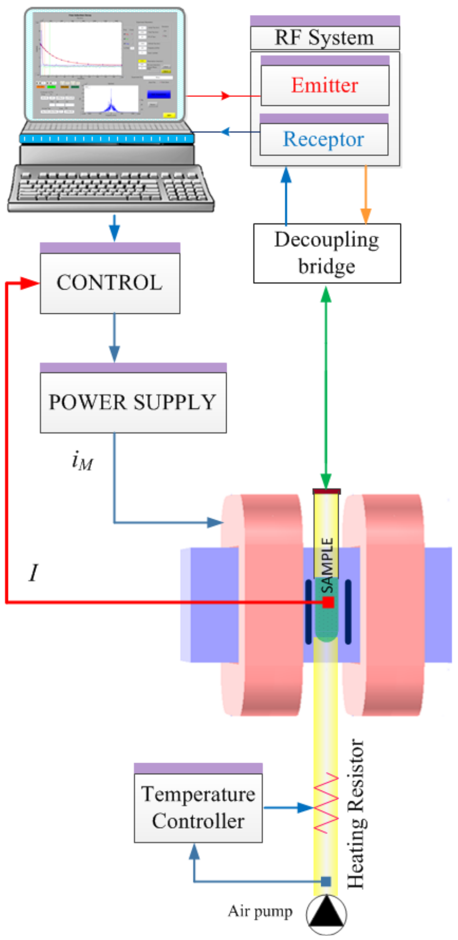

Fig. 1. Main modules of a FFC NMR apparatus.

As main requirement of FFC NMR equipment, the magnet current (i_M) needs to be controlled in order to cycle as shown in Fig. 2.

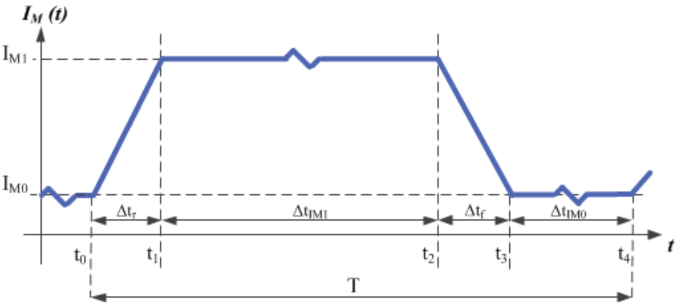

Fig. 2. Typical current cycle of a FFC NMR equipment.

This type of equipment has been designed by teams joining Electrical, Electronic and Physics Engineers, which should have skills in the following topics (Fig. 3):

- Power electronics;
- Electromagnetic devices;
- Control techniques;
- Systems modeling and optimization;
- Experimental techniques and protocols.

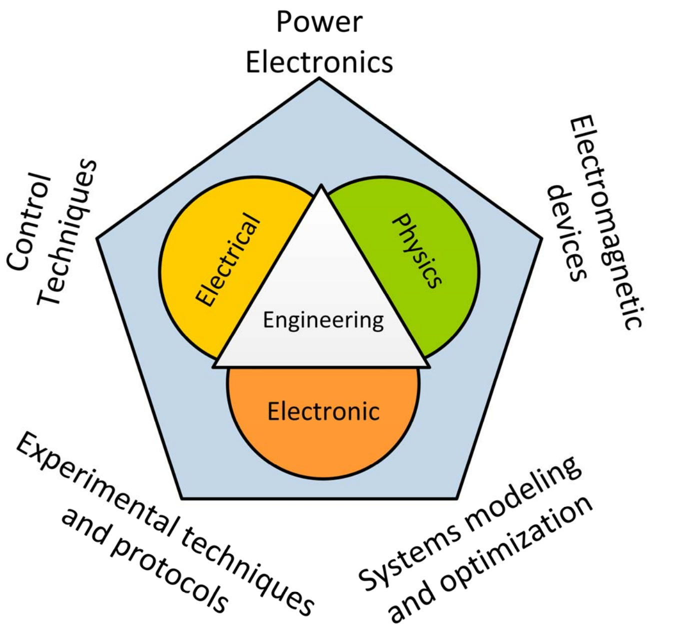

Fig. 3. Main topics related with FFC NMR equipment.

In general, the Electrical and Electronic Engineers are very active during the design and optimization phases. The Physics Engineers have an important role defining the specifications of the equipment, testing and validation phases.

The developed prototypes are, in general, installed in NMR laboratories and have been used by master and PhD students' and senior researchers from different areas, as for instance, physics, chemistry, biology, medical sciences and food industry. Furthermore, it has been also used as a platform to teach electric circuits equipment in Electrical Engineering and Physics Engineering courses.

II. Electric Circuits

One of the core elements of the FFC NMR equipment are the power supplies, which have been improved taking advantage of several technological aspects. Starting with the topologies used at the early days of the technique and crossing the different known solutions [5-11], the FFC NMR power supplies are an effective tool to teach:

- Electric circuits design and analysis (RL, RLC, …);
- Semiconductors (Bipolar transistor, GTO, IGBT, MOSFETS, …).
- Protection circuits.

A circuit implemented in the early days of the FFC NMR technique is shown in Fig. 4. This circuit uses variable resistors to change the magnet current and a switch (S) in order to commute the magnet current.

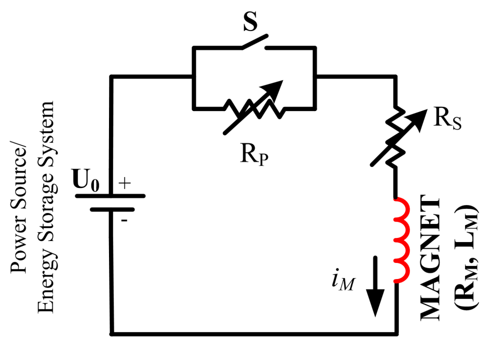

Fig. 4. Electric circuit with variable resistors and a switch.

The electric equation corresponding to the Fig. 4 circuit is:

$$u_0 = \gamma R_P i_M + R_S i_M + R_M i_M + L_M \frac{di_M}{dt} \quad (1)$$

Being,

$$\gamma = \begin{cases} 0 \; if \; S \; is \; OFF \\ 1 \; if \; S \; is \; ON \end{cases} \quad (2)$$

Other circuits and topologies used as power circuits of FFC NMR apparatus are represented in Fig. 5, Fig. 6 and Fig. 7.

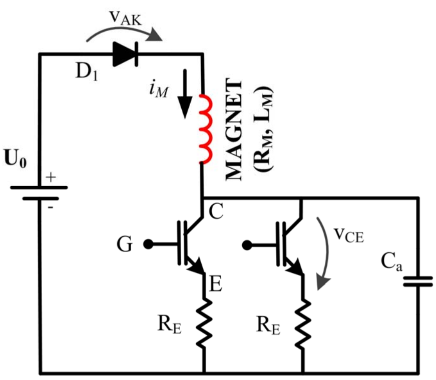

Fig. 5. Electric circuit with semiconductors in parallel.

The solution shown in Fig. 5 is an interesting solution since semiconductors (IGBTs) are placed in parallel. In this case the collector-emitter voltage (V_{CE}) of the IGBT is proportional to the gate-emitter voltage (V_{GE}) in order to control the magnet current. The corresponding electric equation is:

$$u_0 = i_M + L_M \frac{di_M}{dt} + v_{CE} + R_E \frac{i_M}{n} + v_{AK} \quad (3)$$

Where v_{AK} is the drop voltage in the diode D_1 and n is the number of IGBTs in parallel.

In Fig. 6, a topology based on a chopper is shown. This solution had allowed reducing the volume of the existing solutions. This topology was implemented in portable FFC NMR equipment.

In this case, the dynamics of the magnet current depends on the states γ_1 and γ_2 of the switches S_1 and S_2, respectively:

$$\frac{di_M}{dt} = \gamma_1 \frac{U_0}{L} + \gamma_2 \frac{U_{aux}}{L} - (1-\gamma_1)(1-\gamma_2)\frac{R_1}{L} i_M - \frac{R_M}{L_M} i_M \quad (4)$$

Being,

$$\gamma_k = \begin{cases} 1 \ \ if \ \ S_k \ \ is \ \ ON \\ 0 \ \ if \ \ S_k \ \ is \ \ OFF \end{cases} \qquad k = 1,2 \quad (5)$$

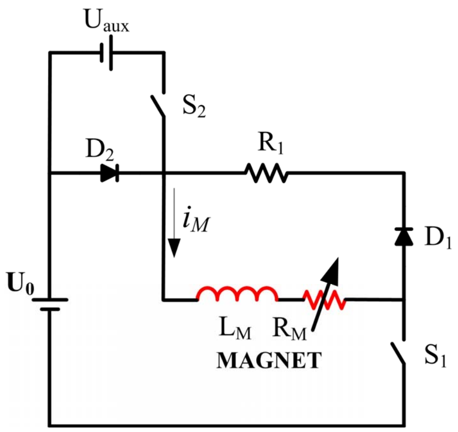

Fig. 6. Solution based on the chopper circuit.

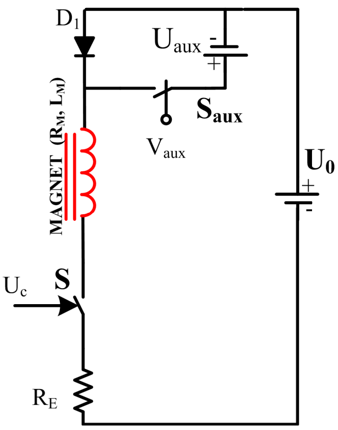

Fig. 7. Solution that can have IGBTs or MOSFETs.

In Fig. 7 is shown the circuit implemented in the most recent prototype. This solution is very similar to Fig. 5, but it requires only a power semiconductor (S) (this solution can use either an IGBT or a MOSFET).

In addition to the referred solutions, FFC NMR power supplies that use GTOs and power bipolar transistors were developed [3].

The solutions based on power semiconductors are also relevant since the power semiconductors require, in general, commutation and protection circuits. A solution based on the circuit in Fig. 7 but including a snubber, a filter and a Zener diode is shown in Fig. 8.

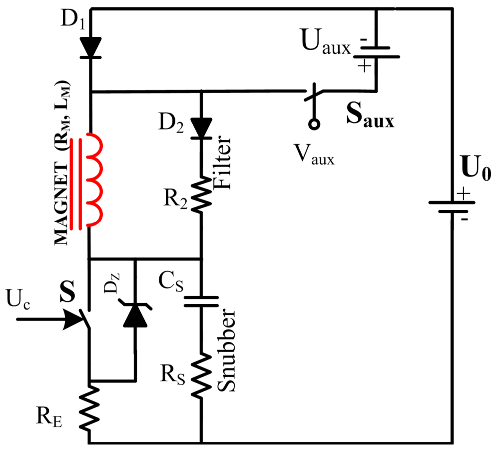

Fig. 8. Solution that can have IGBTs or MOSFETs with protection circuits.

III. Electromagnetic Devices and Optimization Techniques

Other important issue related with the FFC NMR equipment is the magnet design. These magnets can be air-cored solenoids manufactured with aluminum or copper [1-4], [10-11] or can be electromagnets [5-7].

Usually, the design of these magnets requires the knowledge of optimization techniques and programming skills. Two examples of FFC magnets are shown in Fig. 9 and Fig. 10. These solutions are conceptually different and have been taking advantage of materials with distinct characteristics, as for instance, the iron or the copper.

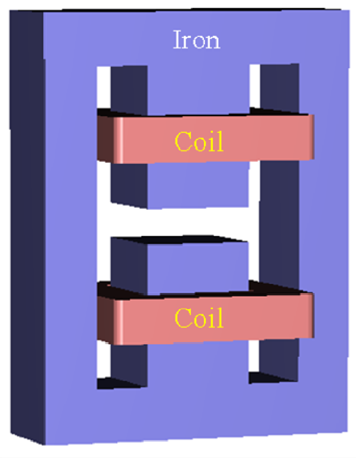

Fig. 9. FFC NMR electromagnet.

Fig. 10. FFC NMR air cored magnet (solenoid type).

As example of the continuous evolution and optimization of FFC NMR magnets, the configuration of a recent solution that includes superconducting parts, is shown, in Fig. 11.

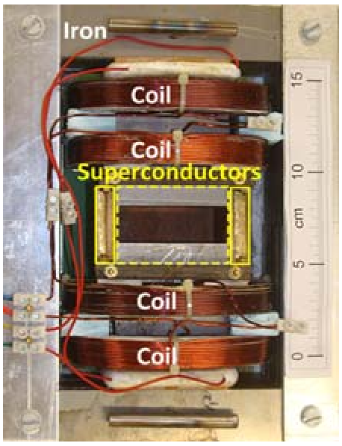

Fig. 11. Electromagnet with superconductors.

About the design of FFC NMR magnets, it is important to refer that this topic can be a useful tool teaching algorithms, optimization techniques and electromagnetic devices. In addition, it is used as an example of a real application that incorporates different materials, which have also distinct electromagnetic properties.

IV. CONTROL

To control the current as required by the application (Fig. 12), different control techniques have been be used [12-14]:

Using as reference the topologies referred in section II, the following types of controllers were implemented:

- PI (proportional and integral actions);
- PD2I (proportional, derivative and two integral actions);
- Two levels hysteretic controller;
- Three level hysteretic controller.

As first approach, for the tuning of the controllers, the generic block diagram represented in Fig. 12 can be used.

Where C(s) represents the controller transfer function and G(s) represents the transfer function of the circuit under analysis (in general, a 2^{nd} or 3^{rd} order system).

To control the current of the circuit represented in Fig. 5, a PI controller was used.

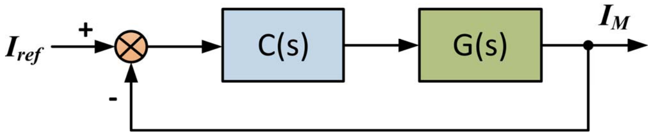

Fig. 12. General control diagram.

Since the Fig. 7 circuit is more complex, a PD2I controller is required. In this case, the circuit can be represented by a 3^{rd} order optimized transfer function:

$$F_{opt}(s) = \frac{b\omega_0^2 s + c\omega_0^3}{s^3 + a\omega_0 s^2 + b\omega_0^2 s + c\omega_0^3} \tag{6}$$

The transfer function of the PD2I controller is:

$$C(s) = k_D k_{I2} \frac{s^2 + \frac{k_P}{k_D} s + \frac{k_{I1}}{k_D}}{s^2} \tag{7}$$

The parameters of the PI and PD2I controllers can be set using ITAE criteria and root loci methods.

For other hand hysteretic controllers, in Fig. 13, were used to control the current of the topology in Fig. 6. In this case, a 3 level hysteretic controller is used, which joins two relays that depend on the current error as represented in Fig. 13.

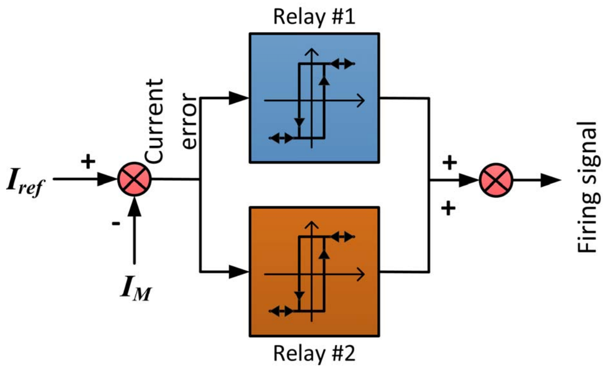

Fig. 13. Block diagram of a three level hysteretic controller.

For the design of the hysteretic controllers, and in order to fulfil the requirements of the application, the methodology considers the effect of changing:

- the maximum switching frequency of the semiconductors;
- the current ripple allowed; and
- the natural time constant of the system (usually imposed by the magnet).

About the controllers, it is important to refer that analog solutions can be found in the existing prototypes. Anyway, during the courses, the students have the opportunity to replace the analog solutions by digital ones based on low cost microcontrollers.

V. CONCLUSIONS AND FINAL REMARKS

In this paper are summarized some aspects and topics used in graduation courses of Electrical Engineering and Physics Engineering based on the evolution of FFC NMR equipment.

Other aspects could be referred, as for instance, the software used to control the equipment and to implement the experimental protocols, experimental procedures, data analysis and data fitting.

Other important aspects addressed in the Electrical and Physics courses are the modeling, simulation and dynamic behavior analysis of electric circuits. In Fig. 14 and Fig. 15, electric circuits that are studied and compared with the circuits represented in Fig. 4 and Fig. 6, respectively, are shown.

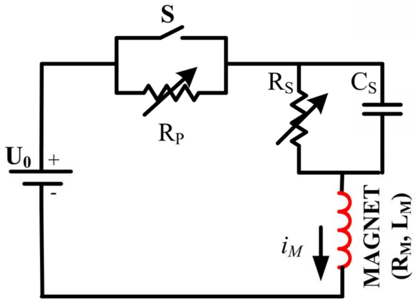

Fig. 14. Electric circuit with variable resistors, a capacitor and a switch.

When analyzing electric circuits, for the circuit in Fig. 14 it is interesting to design the capacitor C_S and to characterize the influence of C_S in the running of this circuit when compared with the solution in Fig. 4.

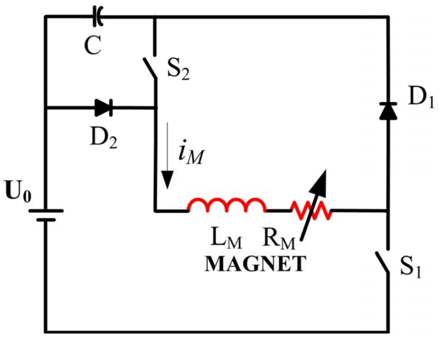

Fig. 15. Solution based on the chopper circuit and energy recovery.

Another important topic that can be taught using the FFC NMR power supplies is the energy recovery. The magnet stores energy that can be used to charge capacitors or batteries (see circuit in Fig. 6, for instance) when the current is stepping down. The stored energy can be reused when the current steps up, improving the global efficiency of the system.

As remark, it is important to point out that the core elements of the FFC NMR equipment, the magnet and the main power supply, has been used in Electrical and Physics Engineering courses of different levels addressing the following topics:

- Electric circuits theory;
- Semiconductors types and operating principles;
- Protection and commutation circuits;
- Electromagnetic devices design;
- Optimization techniques;
- Programming;
- Electromagnetic properties of materials;
- Control techniques;
- Modelization and simulation.

As final remark, in Table I are summarized the number of researchers involved with the FFC NMR technique (using the equipment available at Instituto Superior Técnico – Lisbon) in average per year from 2008 to 2013. About these figures, should be referred that the Electrical Engineering people have been mainly involved in the development and technical improvement of the equipment. The Physics Engineering people have been performing FFC NMR experiments and also contributing to improve this technique. The other people have been only getting experimental results.

TABLE I. NUMBER OF PEOPLE PERFORMING EXPERIMENTS AND/OR DEVELOPMENT OF THE EQUIPMENT (IN AVERAGE PER YEAR – 2008-2013)

	MSc students	PhD students	Senior Researchers
Electrical Engineering	4	1	2
Physics Engineering	5	2	2
Other	4	2	3

For example, the Physics Engineering students have the opportunity to measure parameters related with the molecular dynamics of different compounds. Within the Portuguese context, a typical experiment is performed measuring the spin-lattice relaxation time (T_1) of wines, allowing to check the aging of wines produced in similar conditions (as grapes and soils, for instance), as represented in Fig. 16 [15].

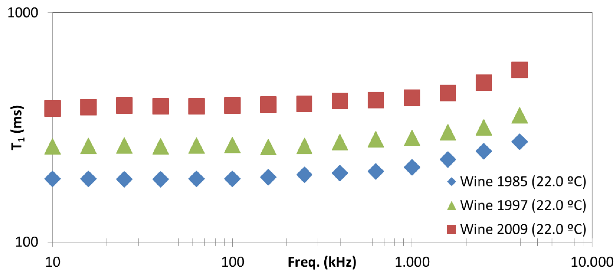

Fig. 16. Spin-lattice relaxation time (T_1) of wines.

ACKNOWLEDGMENT

This work was supported by national funds through *FCT – Fundação para a Ciência e a Tecnologia*, under project PEst-OE/EEI/LA0021/2013.

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