INTRODUCTION

Nuclear magnetic resonance quantum information processing

BY R. M. SERRA1,* AND I. S. OLIVEIRA2

1 Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, R. Santa Adélia 166, 09210-170 Santo André, São Paulo, Brazil
2 Centro Brasileiro de Pesquisas Físicas, Rua Dr. Xavier Sigaud 150, 22290-180 Rio de Janeiro, Rio de Janeiro, Brazil

For the past decade, nuclear magnetic resonance (NMR) has been established as a main experimental technique for testing quantum protocols in small systems. This Theme Issue presents recent advances and major challenges of NMR quantum information processing (QIP), including contributions by researchers from 10 different countries. In this introduction, after a short comment on NMR-QIP basics, we briefly anticipate the contents of this issue.

Keywords: nuclear magnetic resonance; quantum information; quantum computation

1. Introduction

We can attribute the great success achieved so far by nuclear magnetic resonance (NMR) quantum information processing (QIP) to the ability for precisely controlling the dynamics of the nuclear spin system through radiofrequency (RF) pulses. This fine control enables us to construct pulse sequences for preparation of initial states, implementation of quantum gates, simulation of Hamiltonian systems and the determination of system state through quantum state tomography (QST).

An atomic nucleus with nuclear spin ($I = 1/2$) placed in a static magnetic field $B_0$ can encode one qubit of quantum information ($|m_I = +1/2⟩ := |0⟩$, $|m_I = -1/2⟩ := |1⟩$). The Zeeman Hamiltonian of the nuclear qubit is given by $H_Z = \hbar \omega_L I_Z$, where $\omega_L$ is the Larmor frequency and $I_Z$ is the nuclear total angular momentum. Transitions between the energy levels defined by the Hamiltonian $H_Z$ can be induced by the application of oscillating magnetic fields with the appropriate Larmor frequency. The quantum state of the system can be reconstructed from the NMR spectrum, which is obtained by the Fourier transform of the so-called free-induced decay [1].

*Author for correspondence (serra@ufabc.edu.br).

One contribution of 14 to a Theme Issue ‘Quantum information processing in NMR: theory and experiment’.
The simplest prototype of an NMR quantum computer is a two-qubit system described by the (rotating frame) Hamiltonian \[ H = \hbar (\omega_A - \omega) I_A^Z + \hbar (\omega_B - \omega) I_B^Z - \hbar v_A (I_A^X \cos(\phi_A) + I_A^Y \sin(\phi_A)) + \hbar v_B (I_B^X \cos(\phi_B) + I_B^Y \sin(\phi_B)) + 2\pi J I_A^Z I_B^Z. \] (1.1)

The first two terms allow selectivity between qubits \( A \) and \( B \), simply by tuning the RF \( \omega \) to either \( \omega_A \) or \( \omega_B \). The next two terms represent the interaction with the RF field, and allow one-qubit quantum operation. The last term is the so-called \( J \)-coupling between the qubits, and allows two-qubit quantum logical gate implementation. In general, controlled operations can be performed combining different pulse sequences (single-qubit rotations) and free evolution under the \( J \)-coupling. In figure 1, we present an example of a pulse sequence used to employ a control-not (CNOT) gate in a two 1/2-spin system.

One widespread example of a physical system described by this model is the chloroform molecule \( \text{CHCl}_3 \), in which the nuclear \( I = 1/2 \) spins of \( ^{13}\text{C} \) and \( ^1\text{H} \) represent the two-qubit quantum computer.

An interesting variation of an NMR two-qubit quantum computer is the one-spin two-qubit quadrupole system, such as \(^{23}\text{Na} \), which can be described by the Hamiltonian

\[ H = \hbar (\omega_A - \omega) I_Z - \hbar \omega_q I_x + \hbar \omega_Q [3I_Z^2 - I^2]. \] (1.2)

In this case, a nucleus of spin \( I \) and electric quadrupole moment \( Q \) interacts with a static field (first term), an RF field (second term) and an electric field gradient (last term). For \( I = 3/2 \), the Hamiltonian yields a four-level system that can be assigned to two qubits of quantum information. One example of such a system is the sodium dodecyl sulphate. The literature (and this Theme Issue) shows various examples of studies in both cases.

However, an NMR quantum computer does not deal with single molecules, but rather with a sample, which can be a glass tube containing a couple of millilitres of a liquid, with a very large number of molecules. In order for the...
earlier-mentioned Hamiltonians to be a good approximation in a real experimental situation, the ‘quantum computing molecules’ must not interact with each other, a condition that can be achieved by diluting the sample in an adequate solvent. One further difficulty with carbon NMR quantum computers is that $^{13}\text{C}$ is only about 1 per cent abundant. The most abundant $^{12}\text{C}$ has $I=0$. It means that, in a liquid chloroform sample, for instance, only a tiny fraction of the molecules will actually be two-qubit quantum computers, with a huge background of isolated $^1\text{H}$ contributing to the NMR signal. Fortunately, $^{13}\text{C}$-enriched chloroform (and other C-based samples) can be purchased!

The two main facts about NMR-QIP are the following. (i) Thermal equilibrium density matrices can be transformed by means of RF pulses and average techniques to the so-called pseudo-pure states,

$$\rho = \frac{1 - \epsilon}{2^n} I + \epsilon |\psi\rangle\langle\psi|,$$

(1.3)

where $|\psi\rangle$ is a pure state and $\epsilon \approx \hbar \omega / 2nkT$, $n$ the number of qubits and $T$ the equilibrium temperature. The measured NMR signal from such a state is proportional to the nuclear magnetization,

$$M^\pm \propto \text{Tr}\{\sigma^\pm |\psi\rangle\langle\psi|\},$$

(1.4)

therefore behaving as a pure quantum state. (ii) The second point is that RF pulses implement nearly ideal unitary transformation. By exploiting a fine pulse control and free evolution with $J$-coupling, a universal set of quantum logic gates can be designed. Particularly important are pulse sequences that implement the QST, for both spin $1/2$ and quadrupole nuclei [1].

The two earlier-mentioned facts are the very basis of NMR-QIP, and work extremely well for two-qubit quantum computers. But as the number of qubits increases, things rapidly become complicated. One of the main challenges in current research on NMR-QIP concerns the design of special pulse sequences and, for that, powerful techniques have been developed: strong modulating pulses and gradient ascent pulse engineering (GRAPE). In the next paragraphs, we will briefly describe the contents on various aspects of NMR-QIP discussed in this Theme Issue.

A general review about recent advances in NMR-QIP, focusing on decoupling, pulse engineering and indirect nuclear control techniques, is presented by Criger et al. [2]. Souza et al. [3] present a detailed study of a robust dynamical decoupling, which is largely immune to pulse imperfections and enables an increase of the coherence time of the system by several orders of magnitude.

Quantum control is an important part of the quantum technology. Such a topic is reviewed by Schulte-Herbrüggen et al. [4], which illustrates the techniques of quantum control in mixed-state scenarios considering some algorithm classes, such as characterizing the Jones polynomial in order to distinguish between different knots. The quantum control of phases is also the main topic exploited in Simmons et al. [5].

The simulation of quantum systems was one of the first applications of experimental quantum information. Quantum simulations are also interesting to test the advantages of quantum computers over classical ones because the simulating quantum dynamics in classical computers becomes awkward when the system grows. In this context, tests-of-principles have been implemented in NMR
systems with great success. Lu et al. [6] treat such a topic in work focusing particular attention on the possibility to perform quantum chemistry in an NMR simulator.

In the contribution by Modi et al. [7], a simple quantumness witness, in the context of a large number of systems (in a mixed state), is constructed. The authors also discuss the detection of quantumness in NMR-like systems. In a similar direction, the work of Soares-Pinto et al. [8] discusses the quantumness of correlations in NMR systems. In most NMR, implementation of quantum protocol entanglement was ruled out. In this last paper, the authors present some experimental evidence for quantum correlations, and they discuss how non-classical correlations of separable states may be used to simulate quantum dynamics in NMR systems. These two contributions shed some light about quantumness of NMR systems that go beyond the entanglement-separability paradigm.

The tailoring of accurate unitary evolutions is a crucial step in any quantum protocol. The NMR technique uses a sequence composed of pulses especially designed in order to achieve some desired unitary evolution. Ichikawa et al. [9] studied some geometrical aspects of such a composed evolution. They show some possibilities to implement geometric quantum gates in NMR systems. Rowland & Jones [10] review GRAPE pulses to implement quantum logic gates in an NMR quantum processor. They also highlight practical difficulties in implementation due to experimental non-idealities. The GRAPE pulse technique is quite important in NMR scenarios in order to optimize pulses sequences.

An alternative way to process quantum information in NMR systems is to encode multiple qubits in quadrupolar nuclei, which possess a spin greater than 1/2, instead of using multiple two-level systems. Teles et al. [11] present some unique features of quadrupolar systems for QIP. They also review some interesting aspects concerning the relaxation of such systems. Fel’dman et al. [12] discuss the relations between multiple quantum NMR coherences and quantum correlations in solid-state NMR systems considering two exactly solvable models. Also in the context of solid-state NMR systems, Franzoni et al. [13] discuss the utilization of local polarization to storage quantum coherence.

References


