Quantum Computation with NMR

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1 Introduction

A novice seeking to understand Nuclear Magnetic Resonance Quantum Computation (NMR QC) faces a formidable task. Not only is it necessary to master two new fields (NMR and QC), but many of the early papers in the field are unusually difficult to understand. Part of this opacity is, no doubt, due to the speed with which the early manuscripts were written, but an even more important cause was the lack of a common language which would allow NMR experimentalists and QC theoreticians to talk to one another. This barrier is now beginning to be crossed, and more considered pedagogical works are starting to appear.

2 NMR

It is, perhaps, surprising how little known NMR is within the physics community, as it provides a remarkable system for investigating a variety of topics. The name refers to spectroscopic studies of transitions between the Zeeman levels of an atomic nucleus in a magnetic field, and the subject was initially developed by physicists[1, 2] as a method for determining the size of nuclear magnetic moments, and thus testing models of nuclear structure. Within a few years, however, it became clear that measured NMR frequencies were not simply determined by nuclear properties, but also showed a subtle dependence on the properties of the surrounding electronic clouds, and thus on the chemical environment of the nucleus. The messy nature of these "chemical shift" interactions caused most physicists to lose interest, leaving the field to be developed by chemists.

NMR was of obvious interest to chemists as the chemical shift, together with the J-coupling interaction discovered a few years later, provides a powerful method of gaining insights into molecular structure. While other spectroscopic techniques can, perhaps, provide more detailed descriptions of small molecules, NMR is unique in the ease with which it can be applied to complex systems and the remarkably close relationship between the information available from NMR and the mental pictures of molecules used by most chemists. Furthermore, NMR experiments soon reached an extraordinary level of sophistication, involving the systematic generation and interconversion of single and multi spin coherent states. This sophistication was possible as a result of the long coherence times of NMR superpositions, and the exact experimental control possible with RF radiation: similar experiments involving optical transitions have only

become possible in the last few years. These techniques underly modern multi-dimensional experiments, which have enabled NMR to become one of the most important techniques in the molecular sciences.

A vast number of introductory NMR texts are available, but most of these are aimed at chemists or biochemists; such texts typically concentrate on the applications of NMR while avoiding much of the underlying theory. Those texts which are aimed at physicists largely consider NMR studies in the solid state, which have little immediate relevance to current NMR QCs. Fortunately a small number of reasonable texts do exist: the famous text by Ernst *et al.*[3] covers most of modern NMR, and more gentle introductions[4, 5] are also available. It is particularly important to become familiar with the "product operator" description[6], which plays a central role in modern NMR theory.

3 NMR QC

While NMR has largely remained the preserve of chemists, it has occasionally been used to investigate fundamental topics in physics. One notable example is the use of NMR and its close cousin Nuclear Quadrupole Resonance (NQR) to study geometric phases[7, 8]. It has long been known that NMR is in many ways well suited to quantum computation, but early proposals foundered on the difficulty of generating an initial pure state. Most QC schemes rely on cooling to the thermodynamic ground state as an initialisation mechanism, but this approach is not practical within NMR as the energy gap between the Zeeman levels is small compared to kT at any reasonable temperature.

The great breakthrough in NMR QC was the realisation by Cory *et al.* [A] that it is not strictly necessary to form a pure state to implement an NMR QC, as NMR is an ensemble technique in which very large numbers of spins are detected simultaneously (it is not practical to detect the signal from a single spin as a result of the tiny energies involved). Instead it suffices to generate a "pseudo pure" state, that is an ensemble comprising a mixture of the desired pure state and the maximally mixed state. Assembling such a mixture is a fairly conventional problem in NMR, and Cory *et al.* [A] demonstrated all the basic elements required to build an NMR QC; subsequent papers[9, 10] have expanded and clarified many of their ideas. An alternative approach to this problem was subsequently described by Gershenfeld and Chuang[11, 12]; this approach is elegant in principle but complex in practice and has not been widely used. More recently a variety of new approaches have been suggested, among which the method of temporal averaging[13] has proved particularly popular.

Once the initialisation problem had been overcome, progress in the implementation of NMR QCs was rapid. The first algorithm was an implementation of Deutsch's algorithm [B] on a two qubit NMR QC based on the small molecule cytosine; a second implementation based on chloroform[14] was published soon afterwards. These were swiftly followed by two implementations of Grover's quantum search routine; this time the chloroform implementation [C] came first, with the cytosine implementation following behind[15].

While these two early NMR QCs share some common features, there are also some significant differences. Many of these can be traced back to the fact that the cytosine QC uses two ^{1}H nuclei (a *homonuclear* system), while the chloroform QC uses one ^{1}H nucleus and a ^{13}C nucleus (a *heteronuclear* system).

In heteronuclear systems the NMR transition frequencies of the two nuclei are very different, which makes it very easy to distinguish them; in homonuclear systems the frequencies are quite similar, making discrimination between the spins a more challenging problem.

Homonuclear systems do, however, have the advantage that it is possible to address both nuclei simultaneously, and to observe both in the same spectrum, while heteronuclear systems require two completely separate RF channels. This permits a particularly simple readout scheme in homonuclear NMR QCs: it suffices to simply examine the NMR spectrum, in which state $|0\rangle$ is indicated by an absorption, while state $|1\rangle$ appears as an emissive transition. With a heteronuclear system it would be possible to perform two separate detection experiments; alternatively a more detailed analysis of the multiplet structure within the NMR spectrum of one nucleus may be used to characterise the state of the other nucleus. In fact Chuang *et al.* used a total of nine different readout experiments in order to fully characterise the final state of their NMR QC (that is, they performed full quantum state tomography). This gives an excellent idea of the experimental errors involved in their implementation, but tomography is not a practical approach for more general problems, as the number of readout experiments required rises exponentially with the number of nuclei in the system. Furthermore, their implementation uses temporal averaging to produce the initial pseudo pure state, which requires that every experiment be repeated three times. Thus their results represent the combined analysis of 27 separate experiments (although not all these experiments are strictly necessary).

Implementing these small NMR QCs is experimentally quite straightforward, and a number of new systems have been described. Most of these are broadly similar to the two systems described above; in particular multiple pulse techniques are used to modulate the nuclear Hamiltonian, creating an effective Hamiltonian[3] which implements the desired logic gate (this approach has been described in some detail in two recent papers[16, 17]). One three qubit implementation [D], however, adopts a different approach, based on the use of simultaneous line selective pulses. In this method extremely weak RF pulses are used which will excite a nucleus only when the neighbouring nuclei have specific spin states. By this means it is possible to implement several two and three qubit gates directly. This approach is experimentally challenging when applied to homonuclear systems, but may prove useful with heteronuclear implementations.

In addition to these demonstrations of quantum algorithms using NMR QCs, there has also been significant interest in using NMR to demonstrate other phenomena in quantum information processing, such as GHZ states[18, 19], state teleportation[20] and quantum error correction protocols[21, 22]. Some of these topics are related to more conventional NMR ideas, such as multiple quantum coherence and coherence transfer sequences[3], but the language of QC provides an intriguing new view of old concepts.

4 Limitations and problems

From the beginning there has been a strong current of concern regarding the usefulness of NMR QCs; indeed there has been some debate as to whether NMR QCs are in fact *real* QCs. Initial criticism focussed on the question

of scalability[23, 24], and it is now widely accepted that current NMR implementations are probably not scalable for a variety of reasons[25, 26], including the exponential inefficiency in the preparation of pseudo pure states, the limited number of operations which can be carried out before decoherence sets in, and the experimental difficulties involved in implementing logic gates in multispin systems. Despite this somewhat depressing list it should be remembered that NMR is currently well in the lead in implementing small QCs, and that demonstrations involving five qubits[27] and hundreds of gates[28] have been performed. Furthermore, one recent proposal incorporating NMR techniques within a solid state system[29] appears to sidestep these problems.

More recently, it has been suggested[30] that NMR might not be a quantum mechanical technique at all! When assessing this comment, it should be remembered that "quantum mechanical" is used here with a technical meaning of "provably non-classical". As NMR experiments are conducted at temperatures such that kT is large compared with the splitting between the energy levels, the density matrix describing a nuclear spin system is always close to the maximally mixed state, and it can be shown that such high temperature states can always be decomposed as a mixture of product states (that is, states containing no entanglement between different nuclei). As NMR states appear to be describable without invoking entanglement, they can therefore be described using classical models (although these classical models may be somewhat contrived). However, while such classical models can be used to describe an individual NMR state, it is not clear that such models can be used to describe the evolution of the state during an NMR experiment[31]. The significance of these conclusions remains contentious and unclear.

5 Papers

A. **5 pages:** *Nuclear magnetic resonance: an experimentally accessible paradigm for quantum computing,* D. G. Cory, A. F. Fahmy, and T. F. Havel, Proceedings of PhysComp '96 (T. Toffoli, M. Biafore, and J. Leão Eds), 87–91 (1996).

B. **6 pages:** *Implementation of a quantum algorithm on a nuclear magnetic resonance quantum computer,* J. A. Jones and M. Mosca, Journal of Chemical Physics **109,** 1648–1653 (1998).

C. **4 pages:** *Experimental Implementation of Fast Quantum Searching,* I. L. Chuang, N. Gershenfeld and M. Kubinec, Physical Review Letters **80,** 3408–3411 (1998).

D. **7 pages:** *An implementation of the Deutsch–Jozsa algorithm on a three-qubit NMR quantum computer,* N. Linden, H. Barjat, and R. Freeman, Chemical Physics Letters **296,** 61–67 (1998).

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