

**PERSPECTIVE:**

**NMR QUANTUM INFORMATION PROCESSING AND ENTANGLEMENT**

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In this essay we discuss the issue of quantum information and recent nuclear magnetic resonance (NMR) experiments. We explain why these experiments should be regarded as quantum information processing (QIP) despite the fact that, in present liquid state NMR experiments, no entanglement is found. We comment on how these experiments contribute to the future of QIP and include a brief discussion on the origin of the power of quantum computers.

**1. Introduction**

Can we implement QIP using liquid state NMR? At room temperature the nuclear spins of an ensemble of molecules in solution are in a highly mixed state (for a general review of NMR see for instance Ernst et al. [1], and for an overview of its achievements and prospects for QIP see Cory et al. [2]). As the molecules are effectively non-interacting and equivalent, the spin system is described by a density matrix of the form

$$\rho = \frac{1}{2^n} e^{-\beta H} \approx \frac{1}{2^n} (\mathbb{1} - \beta H + \dots), \quad (1)$$

where  $n$  is the number of distinguishable spins in each molecule (*i.e.*, the effective number of qubits),  $H$  is their Hamiltonian, and  $\beta = \hbar/kT$  the inverse thermal energy. The ratio of the energy of the system to the thermal one,  $\beta H$ , is on the order of  $10^{-5}$  (for

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the hydrogen nucleus at 11 Tesla). This implies that the state is extremely mixed, and with the present number of spins (up to seven qubits [3]), it is possible to show that such mixed states are separable [4, 5]. Thus, present day liquid state NMR experiments contains *no* entanglement. If we believed that entanglement was the crucial element for quantum information processing this would be the end of this paper (the shortest one we ever wrote). Indeed it has been quoted in the literature that entanglement is the source of the power of quantum computer [6, 7]. So why are people interested in NMR quantum information technology at room temperature? In this paper we will comment on this question and suggest some answers. We will argue that, at least for small devices, entanglement is not the most important resource for quantum computation (QC), and can even be absent. Nevertheless, as we scale up to large number of qubits, entanglement might become inevitable. We will explore some of the issues related to the apparent power of QC and give arguments why liquid state NMR is an interesting technology for QIP. Two main reasons can be provided: First, because the evolution of the spins is best described by quantum mechanics; Second, because the claim that entanglement is the most important element for QC is only a claim. As such, it should be questioned, and NMR technology is an interesting and experimentally accessible setting that challenges it. Maybe entanglement is needed only asymptotically, and thus would not be necessary for a small number of qubits (this might be the case of the problem of “one-bit” of quantum information discussed below).

Before dwelling further in the discussion, we should remind the reader that there is so far no proof that quantum computers are more powerful than their classical counterparts except in the so-called black box (or oracle) case *i.e.*, when a certain function is evaluated without a detailed circuit for its implementation, and the relevant complexity measure is the number of queries to the oracle. An important example is Grover’s quantum search algorithm [8]. While remaining somewhat unsatisfactory from the physical point of view, such black box models give strong indication that quantum computers are indeed more powerful, but not yet a proof. Even quantum algorithms attaining exponential speed-up, like Shor’s algorithm for quantum factoring [9], are only more efficient than the *known* classical counterpart. This is an important point to keep in mind because the apparent extra power of quantum computers is so far only an assumption. If we would be able to prove that they are more powerful we would probably find, at the same time, the origin of their power.

## 2. Quantum information and entanglement

QC is the manipulation of information using quantum mechanics in order to solve a mathematical problem. This manipulation is local, as opposed to other tasks such as quantum communication which deals with information transmission between separate parties. Unfortunately, we do not have at present a unique definition of the concept of quantum information itself. In the community it has often been associated with the presence of entanglement but this is not always the case (see the notion of discord below).

In the case of quantum communication, where the parties involved can only share specially prepared states, perform local unitary transformations and classical communication, entanglement is an essential part of the protocol, and allows for an improvement of the

channel capacities with respect to their classical values. On the other hand in QC everything is done locally and it is not clear whether entanglement is actually the essential ingredient to improve the efficiency of the computation. As quantum computers seem more powerful than their classical counterpart, we can ask the following question: Is it possible to have quantum information (hence do actual quantum computation!) without having entanglement?

Before we address this question, let us summarize some of the characteristics of entanglement. Pure states are said to be entangled if they cannot be written as product states *i.e.*,

$$|\Psi_{ent}\rangle \neq |\Psi_1\rangle \otimes |\Psi_2\rangle, \quad (2)$$

for the simplest case of a bi-partite system. For mixed states this simple definition fails. A mixed state is said to be entangled if it is non-separable, meaning that it cannot be written as a convex sum of bi-partite states:

$$\rho_{sep} = \sum_i a_i (\rho_1 \otimes \rho_2)_i, \quad (3)$$

where  $\rho_1, \rho_2$  are density matrices for the two subsystems and the non-negative coefficients  $a_i$  are interpreted as classical probabilities. There are interesting physical ensembles which are separable: for example, an equal mixture of all four Bell states can be re-expressed as an equally weighted sum of the states  $|00\rangle, |10\rangle, |01\rangle, |11\rangle$ , which are separable and thus has absolutely no entanglement. This ensemble is made of entangled pairs of qubits but if we do not have the knowledge of the state of each element of the ensemble no entanglement is present anymore. This state remains separable even if there is a small excess of, let's say, the entangled state  $|\Psi_+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$ , such as

$$\rho = \frac{1-\epsilon}{4} \mathbb{1} + \epsilon |\Psi_+\rangle \langle \Psi_+|, \quad (4)$$

as there is another way to construct such density matrix but only with separable states. If the parameter  $\epsilon$  is smaller than  $1/3$  this state is not entangled as it can be rewritten as a state of the form given in eq.(3).

One of the quantitative definitions of the amount of entanglement present in two mixed qubits is related to the amount of pure EPR pairs that can be extracted from copies of the ensemble. This definition of entanglement is based on concepts from quantum communication, not computation.

Entanglement is a new type of resource offered by quantum mechanics which does not have a classical analog (states with entanglement violate Bell inequalities, for example). Although entangled states cannot be used to communicate at distance, they can assist in some communication tasks (for a review see [10]). Indeed, it has been shown by Raz [11] that there is an exponential gap in the amount of resources needed to solve a specific problem if we use entanglement-assisted communication rather than classical communication.

Separable states do not contain the extra correlations which appear in entangled states and are responsible for violating Bell inequalities. It is these correlations that are ultimately exploited in quantum communication. Thus, highly mixed states describing room temperature liquid state NMR (with small number of qubits) could not be used for quantum communication.

To summarize, quantum communication takes advantages of correlations which have no classical counterpart. On the other hand computation is inherently a dynamical process and the relevant resources could, at least in principle, be different.

It seems then reasonable to ask whether there is quantum information in states which are not entangled. There are a few examples of quantum information without entanglement – the work by Bennett *et al.* [12], which demonstrates non-locality without entanglement, and more recently the work by Ollivier and Zurek [13]. The latter is based on the idea of comparing two different definitions of mutual information, obtained by generalizing the classical definition to quantum systems  $X$  and  $Y$ :

$$I(X, Y) = H(X) + H(Y) - H(X, Y), \quad (5)$$

and

$$J(X, Y) = H(X) - H(X|Y). \quad (6)$$

In these equations,  $H(X, Y)$  is the joint entropy of the pair  $(X, Y)$ , while  $H(X)$  and  $H(Y)$  denote the entropies for the reduced states of  $X$ ,  $Y$ , respectively.  $H(X|Y)$  is the conditional entropy of the state of  $X$  given a projection of  $Y$  (summed over a complete set of projections of  $Y$ ). It turns out that  $I$  and  $J$  are equal for classical systems [14], or whenever a joint probability distribution can be constructed for the individual systems  $X$  and  $Y$ . However,  $I$  and  $J$  differ otherwise. Quantum discord is defined as the difference  $D = J(X, Y) - I(X, Y)$ .

An example of a state with non-vanishing discord is any states of the form (4), provided that the measurement involved in (6) is a measurement of  $Y$  alone. Thus, even if these states may have no entanglement, they have a non-zero discord *i.e.*, the information they contain is basically different from classical information. Those kind of states can be reached using generic evolutions in liquid state NMR.

There are other reasons to believe that, indeed, there is more to QIP than just manipulating entangled states. It is an experimental fact that the behavior of nuclear spins in a time scale shorter than the so-called  $T_2$  time is, even at room temperature, surprisingly well described by a unitary evolution. This  $T_2$  time corresponds to the decoherence time where the phase of the state gets randomized. This means that although the system is in a highly mixed state, relative phases are preserved on that time scale. Moreover, we do not have an efficient way to simulate a generic evolution of these systems. So what is it in these evolutions that makes it so hard to simulate? For many years the NMR community has attempted to find classical models to represent the behavior of these high-temperature systems without succeeding (interestingly, this was to a large extent independently rediscovered in the context of QIP, see the work by Shack and Caves [15]). This difficulty is well expressed in a claim by Ernst *et al.* [1]: “The dynamics of *isolated* spins can be understood in terms of the motion of classical magnetization vectors. To describe coupled spins, however, it is necessary to have recourse to a quantum mechanical formalism where the state of the system is expressed by a state function or, more generally, by a density operator” [16].

This is not to say that there are no classical hidden variable theories able to mimic quantum mechanics: one can always construct the hidden variable model which simulates the evolution of the system and arranges the final state to reproduce exactly the quantum

behavior. This is possible as long as the systems is local (*i.e.*, we cannot rule out classical communication between the qubits). This is true not only for highly mixed states but for pure states as well. However these model always seem contrived to a high degree, and assume to some extent that the hidden variables are not counted as resources. If indeed they are not taken into account, then a computer with hidden variables is as good as a quantum computer, although nobody believes that the hidden variables would really be resource-free.

This discussion emphasizes the fact that the distinction between quantum and classical information processing is related to *the amount of resources* used, and not necessarily to the violation of certain criteria such as the Bell inequalities. An algorithm using entanglement does not imply that it is hard to simulate classically as was shown by the example of Knill and Gottesman [17], [18] who realized that the stabilizer operations (the operations which transform tensors product of Pauli operators into tensors product of Pauli operators) can involve highly entangled states, but still states whose information processing capabilities are equivalent to classical ones (this was also noted in [19]). Yet, the most surprising fact about QIP is that it allows for certain algorithms or protocols which are or seem exponentially more efficient.

### 3. Entanglement in NMR experiments

We have emphasized the distinction between quantum and classical information processing through their efficiency at solving problems. It is important to mention that today's liquid state NMR QIP experiments using the present methods for realizing the required pseudo-pure states are not efficient. However Schulman and Vazirani [20] have shown that in the absence of noise there is an efficient algorithm for producing pseudo-pure states. From these efficient pseudo-pure states and the dynamics we could in principle created entangled states. However, with the level of noise and the amount of resources achievable by current technologies, this method remains definitely impractical.

As mentioned in the introduction, no entanglement has been present in room temperature liquid state NMR experiments to date. Nevertheless, the degree of control available on the unitary evolution of the spin ensemble has allowed small algorithms to be demonstrated, clearly showing that quantum features can be implemented in this sort of experiments. The paper of [5] suggests that states might exhibit entanglement at around thirteen qubits – a number possible to reach, in principle, with the existing technology, although creating an entangled state would probably not be enough to motivate such experiment in practice.

There has been solid state NMR experiments where the state is likely to be entangled. The first set is the investigation of so-called multi-coherence or spin counting in calcium fluoride [21]. In this system, it is possible to control the evolution of an out-of-equilibrium state in such a way that after a desired time interval we can label various terms of the density matrix with a magnetic field gradient, and then time-reverse the Hamiltonian with an appropriate series of radio-frequency pulses. The magnetization, which spreads to many nuclei in what the spectroscopists call multi-coherence, can thus be reversed and brought back to its original value with a signature of how large the achieved multi-coherence was. This is done in such a way that operators of the form  $I_+^1 I_+^2 \dots I_+^n$  (where  $I_+ = (\sigma_x + i\sigma_y)/2$

for each spin) acquire a phase which evolves  $n$  times faster than the magnetization of a single spin. These states correspond to pseudo-pure cat-states. Coherences involving at least 60 spins (corresponding to a pseudo-pure cat state of 60 spins), are probably entangled – although nobody has so far provided an analytic proof.

Another type of solid state experiment where entanglement is probably present is the one investigating spin diffusion by Zhang and Cory [22]. In these experiments, the spins of a calcium fluoride crystal are excited and left to interact (diffuse) with their neighbors for some amount of time, and then the evolution is reversed. If the magnetization is initially created locally, it will diffuse through the interaction with neighboring spins, and the relevant question is, At which rate does this happen? Attempts to determine the diffusion rate through classical simulations seem practically unfeasible, as around  $10^{11}$  spins are involved in the quantum dynamics – which would require  $\sim 2^{10^{11}}$  bits of classical memory. With such a large amount of spins involved, the states are probably entangled (but again there is no proof of that yet).

#### 4. On the origin of the power of quantum computers

There have been many suggestions for the origin of the power of quantum computers: the size of the accessible Hilbert space, entanglement, the existence of many universes, and the superposition principle (or quantum interference).

One of the first explanations for the power of quantum computation is the size of the Hilbert space. For example, for  $n$  spin 1/2 particles this size grows as  $2^n$ , thus it is tempting to claim that there is an exponential gain compared to a classical system. But this is easily questionable since the state space of  $n$  classical bits also contains  $2^n$  distinct elements. One step further with this argument is to realize that the quantum system can be in a superposition state. Therefore, although the number of computational basis states is the same in the classical and quantum case, the  $2^n$  computational states exhaust the possible configurations of a classical system, whereas a generic quantum state is specified by an exponentially large set of complex amplitudes along the computational basis. But again we could turn to a probabilistic classical computer (probably a better system to compare to the quantum case) and find that there is an exponential number of states that can have non-zero probability to occur. On the other hand, there are definitely many quantum states which have no corresponding classical analog.

As discussed previously, the presence of entanglement can be invoked to explain the apparent speed up of QC. Ekert and Josza [6] argue that if we start in a pure state and never produce an entangled state we can follow the evolution of the system efficiently using a classical description. A set of classical tops can efficiently simulate a set of qubits which start in a pure state and evolve without entanglement. This can be seen from the Bloch sphere picture, where the state of a qubit is associated to a vector on the sphere. For many pure qubits which never get entangled the state is described as a set of Bloch sphere vectors. These vectors can also be thought of as the directions of the angular momentum of spinning classical tops. Hence transformations that correspond to reaching unentangled pure states can be mimicked by the classical system. However, such a correspondence fails if entangled state are reached, for entangled states cannot be described by a state from a state space obtained by a tensor product of Bloch spheres. The above reasoning

emphasizes the properties of the *state* during a computation.

This argument seems also at first to give convincing evidence of the necessity of entanglement at some stage of the computation – but only if we consider pure states. Difficulties arise if we consider *mixed* states. In this case it is possible to investigate complex evolution operators which keep the state separable. For example, in the case of NMR, evolution operators (*e.g.* C-NOT gates) which would generate entanglement if applied to an initial pure state have been implemented (viewed as the evolution operators of classical tops they lead to negative probability transitions [23]), but because the state is highly mixed no entanglement has been effectively created. However, we would like to also emphasize the amount of information necessary to follow the evolution of the system. In fact, an interesting point is to realize that the power of quantum computers might take its origin in *the properties of the evolution as well as the states it uses* a conclusion which was reached by Caves and Schack [15]. A criteria to distinguish quantum and classical evolution in the context of quantum information processing was given by Poulin [19] Anybody who attempts to simulate these evolutions with present algorithms, quickly realizes that they require an exponential amount of resources as we scale up the simulation (as in the factoring case, however, this does not exclude that we could in the future find efficient methods for such simulations in the future). Another argument against the point made in [6] is the work by Bernstein and Vazirani [24] and also Meyer on so-called sophisticated quantum search without entanglement [25]. They showed that in a black box model it is possible to have a quantum search algorithm that is more efficient than the classical case without requiring entanglement.

Most of the algorithms we know today have a pure initial state, except for possible quantum physics simulations. Motivated by the goal of investigating the origin of the power of NMR QC, the power of one bit of quantum information [26] was studied. The idea was to investigate what could be done with one qubit in a pseudo-pure state while all other qubits are in completely mixed state (unit density matrix). After a Hadamard gate and a control operation, the expectation value of the operator  $\sigma_x$  of the first qubit in the circuit of Fig. 1 is given by

$$\langle \sigma_x^1 \rangle = \frac{\epsilon}{2^{n-1}} \text{Re Tr}[U], \quad (7)$$

where Re and Tr denote the real part and the trace operation, respectively. Choosing the state of the  $n - 1$  last qubits to be proportional to the identity density matrix gives us an efficient way to find the trace of any unitary operator  $U$  which is efficiently implementable (there is a factor of  $1/2^{n-1}$  in the density matrix but the trace is a sum over  $2^n$  numbers). From a classical point of view this algorithm makes little sense, as most of the bits are in a completely random state. But for quantum systems, phases between states can be manipulated even in the presence of highly mixed states as long as decoherence is negligible. As is the case of factoring, calculating the trace of an operator  $U$  of the form  $e^{-iHt}$  (for a generic physical Hamiltonian  $H$ ) is a difficult task classically.

The attractive feature of this computation is that the initial state required for the quantum algorithm is scalable using the high temperature limit of a thermal state. The state is obtainable by removing the polarization on all qubits except a single one. Thus, in the absence of noise, there is at least one (non black box) quantum algorithm with no

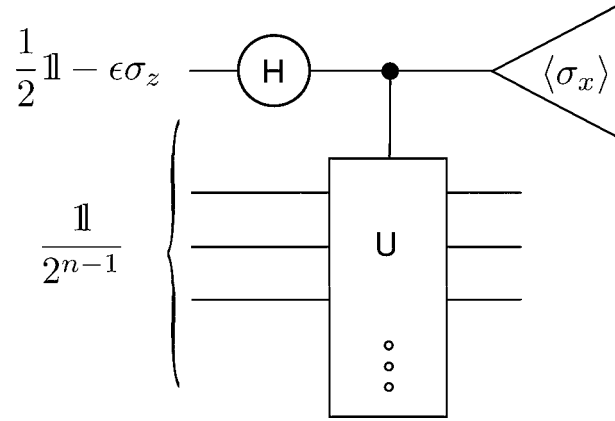


Fig. 1. Quantum circuit evaluating the real part of the trace of the operator  $U$  from an initial state of the form  $\frac{1}{2^{n-1}}(\frac{1}{2}\mathbb{1} - \epsilon\sigma_z) \otimes \mathbb{1}$ .  $H$  represents the Hadamard gate.

known efficient classical counterpart. For thermal states with little polarization, there will be no entanglement for a small number of qubits. For fixed polarization, entanglement might appear for some threshold number of qubits, but there is no indication to believe that at this number anything special occurs, or the efficiency of the algorithm dramatically changes. This algorithm thus questions the claim that entanglement is essential for speed-up.

An interesting point about the argument on entanglement is that it implicitly relies on some notion of locality and an assumption on how the physical system representing the qubits is behaving. After all we could think of having a single quantum system with  $2^n$  dimensions and having the gates globally acting on these states, thus mimicking operations on entangled states; why shouldn't physics allow this control? In other words, the notion of entanglement is *basis-dependent*, *i.e.* relative to a preferred subsystem decomposition, and the relevant question is how that basis is chosen [27, 28].

A third possibility is that the power of quantum computers originates in the interference of the so-called multi-verse [29]. Even if some people find this suggestion compelling, it would be hard to prove or disprove such hypothesis.

A final suggestion is that the essential ingredient is the superposition principle of quantum mechanics. The first consequence of this principle is the size of the accessible Hilbert space; we already discussed this point. The second consequence is that the quantum superpositions interfere. At first sight it would appear that classical wave mechanics also allows superposition and interference, so could we use water waves to quantum compute? The answer seems to be no, because there are superpositions that have no classical analog.

Maybe in the end we will learn that we need a combination of several of these resources or that different resources are exploited for different approaches to obtain additional power from quantum mechanics. Another possibility is the impossibility to separate superposition, quantum dynamics, entanglement, projective measurement for a scalable quantum device and that all these ingredients are important even though a dissection is necessary



to arrive at this conclusion. By exploring concrete examples of QIP we hopefully will learn about the essence of quantum computation.

## 5. Conclusion

In this essay we provided partial answers to the followings questions:

- Is entanglement required to have quantum information?
- Is entanglement responsible for the apparent power of QC or is it incidental?
- What is the origin of such power?

We argued that there is more to QIP than just the creation and manipulation of entangled states, and commented upon the recent suggestion by Ollivier and Zurek to relate quantum information to discord. We also described some solid state experiments where entanglement is probably present. Finally, it is worth stressing that because we still do not know the exact origin of the power of QC, we do not know its necessary ingredients. However, it seems that the superposition principle and a state space dimensionality which grows exponentially with the number of systems used should be part of the requirements.

Having said this, we believe it is important to remind the reader that the authors do understand the limitations of liquid state NMR experiments, while at the same time they are convinced that these experiments provide a well-definite and accessible test bed for some of the ideas of QIP. One achievement of the NMR community has been to demonstrate control of generic unitary transformations constructed from a set of universal gates (for example, some of the work by Waugh and collaborators [30] was well before the interest in QC). This is a fundamental contribution to the field of QIP. Another fundamental contribution is the study of error mechanisms, which shows that the actually occurring errors seem to be reasonable enough to be compensated for by quantum error correction – at least in the sense that the relevant error models are of the type expected, although the error magnitude is still too high for error-correcting and fault-tolerant methods to be fully effective. In spite of this, it has been possible to show that the unitary control is able to take into account errors due to a variety of sources, such as mis-calibration, off-resonance, and inhomogeneity, and that gate fidelities better than 0.999 can be currently achieved [31]. This also shows how important types of coherent errors can be controlled efficiently without having to recourse to full quantum error correction.

A further contribution is the knowledge acquired while translating ideal quantum circuits into physically realizable ones. As ideal circuits often assume some gates or operations which are not directly available in a specific implementation, finding ways to circumvent these limitations is an important step forward. Moreover, the study of scalability even for rather small numbers of qubits (two to seven) already indicates some of the difficulties encountered in going to larger numbers of qubits. With two or three qubits, it is straightforward to design a pulse sequence which implements a certain algorithm while minimizing some of the imperfections of the device, but with five to seven it is much more challenging, and automation becomes necessary. Understanding the optimal way to do this will be crucial for any device which goes beyond a few qubits.

Finally, the present liquid state NMR experiments open the way for a second generation of experiments: the solid state ones. They will also have their limitations, but we hope

they will allow a better understanding of some of the difficulties of building QIP devices and to find ways to overcome them.

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