

NMR Implementation of a Building Block for Scalable Quantum Computation

D.E. Chang ^{a,c,1}, L.M.K. Vandersypen ^{b,c,*}, M. Steffen ^{b,c,2}

^a*Stanford University, Department of Physics, Stanford, CA 94305*

^b*Stanford University, Department of Electrical Engineering, Stanford, CA 94305*

^c*IBM Almaden Research Center, San Jose, CA 95120*

Abstract

We report the implementation of the central building block of the Schulman-Vazirani procedure for fully polarizing a subset of two-level quantum systems which are initially only partially polarized. This procedure consists of a sequence of unitary operations and incurs only a quasi-linear overhead in the number of quantum systems and operations required. The key building block involves three quantum systems and was implemented on a homonuclear three-spin system using room temperature liquid state nuclear magnetic resonance (NMR) techniques. This work was inspired by the state initialization challenges in current NMR quantum computers but also shines new light on polarization transfer in NMR.

1 Introduction

The possibility of constructing computers that operate based on the laws of quantum physics has been raised by a series of theoretical results over the last twenty years [1–3]. Compared with classical computers, the promise of these quantum computers lies in their potential ability to solve a wider class of problems “efficiently” — that is, without incurring an overhead in time or physical resources that increases exponentially with the problem size. Several recent experiments brought this theory into practice using liquid-state NMR techniques, with coupled nuclear spins as quantum bits (qubits). In these

* Corresponding author. E-mail: lieven@snow.stanford.edu

¹ E-mail: dchang@snow.stanford.edu

² E-mail: msteffen@snow.stanford.edu

implementations, the spin-up and spin-down states represented the computational basis states $|0\rangle$ and $|1\rangle$ [4–9]. This work for the first time demonstrated the feasibility of small-scale quantum computers.

A characteristic feature of nuclear spin systems in equilibrium at moderate temperatures is that the spin polarization is typically only about 10^{-5} to 10^{-6} . In other words, the spins are in a highly random or *mixed* initial state, whereas the desired initial state for quantum computation is a well-known or *pure* state. The ability to perform quantum computation with a mixed initial state derives from methods to create *effective pure* states [4,5]; these are mixed states which produce the same signal, up to a scaling factor, as spins in the corresponding pure state. The preparation of effective pure states, however, is inefficient: the resulting signal strength decreases exponentially with the number of qubits k [4,5]. Clearly, preparing effective pure states in this way is not a scalable approach to quantum computing.

Very high polarizations could be achieved by cooling the liquid NMR sample down to the milli-Kelvin regime, but this would freeze the sample, reintroducing dipolar couplings and resulting in very broad lines and short coherence times, which is problematic for quantum computing. Several proposals exist to address these complications [10,11], but their feasibility and scalability remain to be demonstrated. Other physical cooling methods could be used to increase the initial polarization. The use of optical pumping [12] is promising, but the state of the art (in liquid state) is still far removed from generating highly polarized nuclear spins useful for quantum computation. Two proton spins have recently been hyperpolarized using *para* hydrogen and subsequently used in a quantum computation [13], but scaling to k qubits requires precursor molecules which easily react with $k/2$ H_2 molecules to form a stable quantum computer molecule. It is unlikely that any of these techniques in themselves will provide large-scale quantum computers.

Remarkably, an *algorithmic* — and thus technology independent — solution to the state initialization problem was recently developed by Schulman and Vazirani [14] (a related but less efficient algorithm was devised earlier by Cleve and DiVincenzo [15] in the context of Schumacher compression). Their initialization procedure is based upon polarization transfer and allows one to fully polarize k qubits starting from n ($> k$) partially polarized qubits. Polarization transfer is widely utilized in the NMR community and the bounds on the achievable polarization enhancements have been well documented [16,17]. The contribution of Schulman and Vazirani lies in the development and analysis of an explicit algorithm for polarization enhancement which asymptotically (for large k) approaches the entropy bound and does so *in a runtime quasi-linear in k and using a total number of spins n which is linear in k* . Since the overhead is only polynomial in k as opposed to exponential in k , this algorithm makes the initialization of room temperature NMR quantum computers, and

of any quantum computer which starts from “high temperature” qubits, in principle scalable.

In this letter, we report the experimental realization of the key step of the Schulman-Vazirani scheme using liquid state NMR techniques. The experiment was performed on a homonuclear three-spin system, for which eigenvalue conservation allows a maximum polarization enhancement factor of $3/2$.

2 Theoretical bounds on polarization transfer

Let us define the polarization ϵ of a spin j as the difference in probabilities between the spin up and spin down state, tracing out the other spins in the molecule. Mathematically, this is expressed as $2\text{Tr}(\tilde{\rho}I_z^j)$, where $\tilde{\rho}$ is the density matrix of the spin system and I_z^j is the usual angular momentum operator of spin j in the \hat{z} direction. So spin j is in the ground state $|0\rangle$ with probability $\frac{1+\epsilon}{2}$ and in the excited state $|1\rangle$ with probability $\frac{1-\epsilon}{2}$.

In thermal equilibrium at room temperature, the polarization $\epsilon = \epsilon_0$, where $\epsilon_0 = \hbar\omega/2kT$ is a very small number, about 10^{-5} to 10^{-6} for typical magnetic field strengths, because the thermal energy kT is much larger than the energy difference $\hbar\omega$ between the spin up and spin down state. We will from now on associate a temperature with the polarization of a spin: a spin with relatively high polarization is considered “cold”, while one with low polarization is considered “warm”.

The polarization of one or more spins can be increased reversibly by polarization transfer from the remaining spins in the same molecule via a sequence of RF pulses and delay times. The maximum polarization enhancement that can be achieved reversibly is bounded by entropy considerations. Specifically, all reversible procedures, such as pulse sequences with negligible relaxation, must conserve the entropy, given by $H = -\text{Tr}(\tilde{\rho} \log \tilde{\rho})$. However, bounds established using entropy conservation are often weak [16], and a stronger universal bound on spin dynamics must be considered.

The spin dynamics bound on polarization enhancement derives from eigenvalue conservation of the density matrix, a second necessary condition for reversibility. This bound can be calculated via the deviation density matrix ρ , where $\tilde{\rho} = 1/2^n(I + 2\epsilon_0\rho)$ (note that the polarization $2\text{Tr}(\tilde{\rho}I_z^j)$ is proportional to $2\text{Tr}(\rho I_z^j)$, since I_z is traceless). By convention in NMR and for the sake of simplicity, subsequent use of the term “density matrix” will actually refer to ρ . Suppose that we have an initial density matrix ρ_i , and we seek to transform it into some final density matrix A , which may be unachievable when using only unitary operations. We then wish to find among all the achievable final

density matrices ρ_f the one that is “closest” to A — that is, whose mathematical projection onto A is maximized. Equivalently, we wish to maximize the coefficient a in the following expansion of ρ_f :

$$\rho_f = aA + bB, \quad (1)$$

where B represents a matrix orthogonal to A , so that $\text{Tr}(A^\dagger B) = 0$. It can be shown [16] that

$$a^{max} = \frac{\text{Tr}(\rho_i^D A^D)}{\text{Tr}(A^2)}, \quad (2)$$

where ρ_i^D and A^D are diagonalized representations of A and ρ_i , with the diagonal elements arranged in descending order from left to right. When both ρ_i and A are already diagonal, evaluation of (2) is particularly simple, reducing to a rearrangement of the diagonal elements and a trivial trace calculation.

For a homonuclear three-spin system starting from thermal equilibrium at room temperature ($\epsilon = \epsilon_0 \ll 1$), the initial density matrix can be expressed as $\rho_i = I_z^a + I_z^b + I_z^c$, or in explicit matrix form,

$$\rho_i = \frac{1}{2} \begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3 \end{pmatrix}. \quad (3)$$

If the goal is to maximize the polarization of spin a , the desired final density matrix is $A = I_z^a$. Application of (2) then readily yields a maximum possible projection $a^{max} = 3/2$ onto A . Since the projection of ρ_i onto A yields $a^{initial} = 1$, the maximum achievable polarization enhancement factor starting from thermal equilibrium is $a^{max}/a^{initial} = 3/2$.

3 The Schulman-Vazirani Scheme

The bounds on polarization transfer established more than ten years ago indicate that unitary polarization transfer procedures could in principle result in very high polarization enhancements [16]. However, only recently, due to the work of Schulman and Vazirani, did an *explicit and efficient* unitary procedure become available for transforming the thermal equilibrium state into a

state in which a subset of the spins exhibits a polarization that asymptotically approaches $\epsilon = 1$ [14]. This procedure was originally invented to initialize the spins in NMR quantum computing in a scalable way, but it can be used to efficiently boost the polarization of any subset of a set of partially polarized qubits, regardless of their physical implementation as long as the available Hamiltonians can generate the necessary unitary transformations.

The idea behind the Schulman-Vazirani scheme is to redistribute the entropy over the qubits, such that the entropy of a subset of the qubits approaches zero while the entropy of the remaining qubits increases and the total entropy is preserved. The following “boosting procedure” (summarized in Fig. 1) serves as the building block for this polarization transfer scheme [14]:

Given three qubits a, b , and c with identical initial polarizations $\epsilon = \epsilon_0$, the initial state $|x_a\rangle \otimes |x_b\rangle \otimes |x_c\rangle$, or for short $|x_a\rangle|x_b\rangle|x_c\rangle$, is one of the eight possible states $|0\rangle|0\rangle|0\rangle, |0\rangle|0\rangle|1\rangle, \dots, |1\rangle|1\rangle|1\rangle$, with respective probabilities $(\frac{1+\epsilon_0}{2})^3, (\frac{1+\epsilon_0}{2})^2(\frac{1-\epsilon_0}{2}), \dots, (\frac{1-\epsilon_0}{2})^3$.

First perform a CNOT operation (Table 1) on c conditioned on the state of b . The new state of the three qubits is $|x'_a\rangle|x'_b\rangle|x'_c\rangle = |x_a\rangle|x_b\rangle|x_b \oplus x_c\rangle$, where \oplus denotes addition modulo 2. Note that *conditioned* on $|x'_c\rangle = |0\rangle$, the polarization of b is now $\frac{2\epsilon_0}{1+\epsilon_0^2}$ (b is almost twice as cold as before); *conditioned* on $|x'_c\rangle = |1\rangle$, the polarization of b is 0 (b is at infinite temperature). However, *overall*, the polarization of b is still the same as before, ϵ_0 . The polarization of a is of course also still ϵ_0 . We then perform a NOT operation on c followed by a Fredkin gate (Table 1) with c as the control qubit. The result is that a and b are swapped if and only if $|x'_c\rangle = |0\rangle$ (and thus if and only if b has been cooled): $|x''_a\rangle|x''_b\rangle|x''_c\rangle = |x'_b\rangle|x'_a\rangle|x'_c\rangle$ if $|x'_c\rangle = |0\rangle$, and $|x''_a\rangle|x''_b\rangle|x''_c\rangle = |x'_a\rangle|x'_b\rangle|x'_c\rangle$ otherwise. On average, a will thus be colder than before. The resulting polarization of a is $\epsilon = \frac{3\epsilon_0}{2} + \mathcal{O}(\epsilon_0^3)$, where the higher order terms are negligible, so the polarization of spin a is enhanced by a factor of $3/2$.

In order to achieve increasingly higher polarizations, this boosting procedure must be applied repeatedly, whereby a fraction of the cold spins obtained from one round is made progressively colder in the next. Spins of little or no polarization are discarded in each round. Analyzing the polarization transfer using energy and temperature considerations, Schulman and Vazirani demonstrated [14] that the progression of rounds can be arranged so that k bits with nearly optimal enhancement can be extracted. Specifically, the theoretical maximum k_{max} of zero temperature ($\epsilon = 1$) bits that can be extracted is given by the entropy bound:

$$k_{max} = (1 - H(\epsilon_0))n, \quad (4)$$

where

$$H(\epsilon) = -\frac{1+\epsilon}{2} \log_2 \frac{1+\epsilon}{2} - \frac{1-\epsilon}{2} \log_2 \frac{1-\epsilon}{2}, \quad (5)$$

and ϵ_0 is the initial polarization. Under the Schulman-Vazirani scheme (and in agreement with the bounds of Ref. [17]), as $n \rightarrow \infty$, the actual number of extracted qubits $k \rightarrow k_{max}$, and their polarization $\epsilon \rightarrow 1$. Furthermore, the number of elementary operations (pulses and delay times in NMR) required to accomplish the entire process is only $\mathcal{O}(n \log n)$. In summary, the initialization scheme is optimal (it reaches the entropy bound) and efficient (k is proportional to n , and the runtime is quasi-linear).

4 Implementation of the boosting procedure

The quantum circuit of Fig. 1, which summarizes the steps in the Schulman-Vazirani boosting procedure, results in the unitary operation (with a the most significant qubit)

$$U = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad (6)$$

which transforms the thermal density matrix as

$$I_z^a + I_z^b + I_z^c \rightarrow \frac{3}{2} I_z^a + \frac{1}{2} I_z^b - I_z^a I_z^c - I_z^b I_z^c. \quad (7)$$

The propagator U thus redistributes the populations in such a way that the highest populations are moved to states with $|a\rangle = |0\rangle$. This can be clearly seen by expressing the resulting density matrix in explicit matrix form:

$$\rho_f = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3 \end{pmatrix}. \quad (8)$$

Because the density matrix remains in a diagonal state after application of each quantum gate in Fig. 1, the boosting procedure can actually be implemented using a simplified quantum circuit: replacing each gate with a gate whose unitary matrix is correct up to phases preserves the transformation given by (7). Consequently, the Toffoli gate, for which the fastest known implementation takes on the order of $7/4J$ seconds (taking all J_{ij} to be $\approx J$), can be substituted with a Toffoli gate correct up to phases — consisting of a $90^\circ \hat{y}$ rotation of b when c is in $|1\rangle$, followed by a $180^\circ \hat{z}$ rotation of b when a is in $|1\rangle$ and a $-90^\circ \hat{y}$ rotation of b when c is in $|1\rangle$ — which takes only $1/J$ seconds. The actual pulse sequence used in the experiment is given in Fig. 2. This sequence was designed by standard pulse sequence simplification techniques supplemented by Bloch-sphere intuition. The resulting unitary operator is

$$\tilde{U} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (9)$$

5 Experimental results

A 2 mol % solution of C_2F_3Br in deuterated acetone was used as the homonuclear three-spin system, for its remarkable spectral properties: strong chemical shifts (0, 28.2, and 48.1 ppm, arbitrarily referenced) and large scalar couplings ($J_{ab} = -122.1$ Hz, $J_{ac} = 75.0$ Hz, and $J_{bc} = 53.8$ Hz) combined with long relaxation times (T_2 's ≈ 4 -8 s). The experiments were conducted at $30.0^\circ C$ and 11.7 Tesla, on a Varian ^{UNITY}INOVA spectrometer.

All pulses were spin-selective, and varied in duration from 1 to 3 ms. “Hermitite 180” [18] and “av90” [19] shaped pulses were employed for 180° and 90° rotations respectively, in order to minimize the effect of the J couplings between the selected and non-selected spins during the pulses. Couplings between the unselected spins are irrelevant whenever those spins are along $\pm\hat{z}$. Bloch-Siegert shifts [20] were accounted for in the pulse sequence out of necessity: they result in an extra phase acquired by the non-selected spins in their respective on-resonance reference frames. These phase shifts are in some cases more than 90° per pulse, while even phase shifts on the order of 5° are unacceptable. For simplicity, Bloch-Siegert corrections and other \hat{z} rotations were implicitly performed by changing the phase of subsequent RF pulses. The duration of the entire sequence of Fig. 1 is about 70 ms.

The theoretical predictions for the spectrum of each spin after the boosting procedure can be derived most easily from (8), taking into account the sign and magnitude of the J -couplings. After a readout pulse on spin a , the four spectral lines in the spectrum of a should ideally have normalized amplitudes 1 : 2 : 1 : 2, compared to 1 : 1 : 1 : 1 for the thermal equilibrium spectrum (for spins b and c , the boosting procedure ideally results in normalized amplitudes of 0 : 1 : 0 : 1 and $-1 : 0 : 0 : 1$, respectively). So the prediction is that the boosting procedure increases the signal of spin a averaged over the four spectral lines by a factor of $3/2$, equal to the bound for polarization enhancement established in Section 2.

The experimentally measured spectra before and after the boosting procedure are shown in Fig. 3. Clearly, the signal of spin a has increased on average as a result of the boosting procedure, and the relative amplitudes of the four lines are in excellent agreement with the theoretical predictions. The measured areas under the four peaks combined before and after polarization transfer have a ratio of 1.255 ± 0.002 . The spectra of spins b and c after the boosting procedure are also in excellent agreement with the theoretical predictions, up to a small overall reduction in the signal strength. The proper operation of the boosting procedure is further validated via the experimentally measured density matrix (Fig. 4), which demonstrates not only that the boosting procedure exchanges the populations as intended, but also that it doesn't significantly excite any coherences. The experimentally measured $\text{Tr}(\rho_f I_z^a) / \text{Tr}(\rho_i I_z^a)$ gives a polarization enhancement factor of 1.235 ± 0.016 , consistent with the enhancement obtained just from the peak integrals of spin a . The experimental implementation of the boosting procedure thus successfully increased the polarization of spin a .

Despite the excellent qualitative agreement between the measured and predicted data, the quantitative polarization enhancement of spin a is lower than ideally achievable. Given the absence of substantial coherences (Fig. 4), we attribute this suboptimal enhancement primarily to signal attenuation due to RF field inhomogeneity and, to a lesser extent, due to transverse relaxation. The minor excitation of coherences is attributed mostly to incomplete removal of undesired coupled evolution during the RF pulses.

6 Summary

We have experimentally demonstrated the building block for the hyperpolarization procedure outlined by Schulman and Vazirani on a homonuclear three-spin system. However, the repeated boosting required in a much larger spin system would be counteracted by relaxation and other causes of signal decay, such as RF field inhomogeneity. Also, it should be noted that when starting from thermal equilibrium at room temperature, the overhead in the number

of nuclear spins required for the complete Schulman-Vazirani scheme is enormous [14], despite its linear scaling: with $\epsilon_0 \approx 3 \times 10^{-5}$, at most one out of every 10^9 spins in a molecule can be fully polarized. Yet, the Schulman-Vazirani scheme could become practical for enabling scalable quantum computation in conjunction with other techniques which increase the initial polarization, or in other quantum bit implementations with higher initial polarizations.

Our implementation and discussion of the Schulman-Vazirani scheme also shines new light on polarization transfer bounds and techniques in NMR. The polarization of one of three spins was boosted using an explicit and general protocol for achieving optimal polarization transfer in arbitrary spin systems. By analysis of energy and temperature limits, it has been shown that this protocol asymptotically achieves the entropy bound as $k \rightarrow \infty$ and does so *efficiently*, i.e. without incurring any exponentially growing overhead.

7 Acknowledgements

We thank C.S. Yannoni for preparing the sample, I.L. Chuang, O.W. Sørensen, and T. Schulte-Herbrüggen for useful discussions, X. Zhou for helpful comments to the manuscript and W. Risk and J.S. Harris for support. LV gratefully acknowledges a Yansouni Family Stanford Graduate Fellowship. This work was supported by DARPA under the NMRQC Initiative.

References

- [1] R.P. Feynman, Int. J. Theor. Phys. 21 (1982) 467.
- [2] D. Deutsch, Proc. R. Soc. London, Ser. A 400 (1985) 97.
- [3] P.W. Shor, Proc. 35th Ann. IEEE Symp. on Found. of Computer Science (1994) 124.
- [4] N.A. Gershenfeld and I.L. Chuang, Science 275 (1997) 350.
- [5] D.G. Cory, A.F. Fahmy, and T.F. Havel, Proc. Natl. Acad. Sci. USA 94 (1997) 1634.
- [6] I. L. Chuang, L.M.K. Vandersypen, X. Zhou, D.W. Leung, S. Lloyd, Nature, 393 (1998) 143.
- [7] J.A. Jones and M. Mosca, J. Chem. Phys. 109 (1998) 1648.
- [8] L.M.K. Vandersypen, M. Steffen, G. Breyta, C.S. Yannoni, R. Cleve and I.L. Chuang, Phys. Rev. Lett. 85 (2000) 5452.

- [9] For a review, see J.A. Jones, Fortschr. Phys. 48 (2000) 909.
- [10] D.G. Cory et al., Fortschr. Phys. 48 (2000) 875.
- [11] T. D. Ladd, J. R. Goldman, A. Dana, F. Yamaguchi, Y. Yamamoto, see <http://xxx.lanl.gov/abs/quant-ph/0009122>.
- [12] R.J. Fitzgerald, K.L. Sauer, W. Happer, Chem. Phys. Lett. 284 (1998) 87.
- [13] P. Hubler, J. Bargon, S. Glaser, J. Chem. Phys. 113 (2000) 2056.
- [14] L. Schulman and U. Vazirani, Proc. 31st ACM Symp. on Theory of Computing (1999) 322.
- [15] R. Cleve and D.P. DiVincenzo, Phys. Rev. A 54 (1996) 2636.
- [16] O.W. Sørensen, Progress in NMR Spectroscopy 21 (1989) 503.
- [17] O.W. Sørensen, J. Magn. Reson. 93 (1991) 648.
- [18] W.S. Warren, J. Chem. Phys. 81 (1984) 5437.
- [19] D. Abramovich and S. Vega, J. Magn. Reson. A 105 (1993) 30.
- [20] L. Emsley and G. Bodenhausen, Chem. Phys. Lett. 168 (1990) 297.

NOT		CNOT		Fredkin		Toffoli	
in	out	in	out	in	out	in	out
0	1	00	00	000	000	000	000
1	0	01	01	001	001	001	001
		10	11	010	010	010	010
		11	10	011	011	011	011
				100	100	100	100
				101	110	101	101
				110	101	110	111
				111	111	111	110

Table 1: Truth tables for the NOT, controlled-not (CNOT), controlled-swap (Fredkin), and doubly controlled-not (Toffoli) operations. The NOT operation flips an individual qubit. The CNOT gate flips the “target” qubit if the control qubit is 1. The Fredkin gate swaps two qubits conditional on the control qubit being 1. In this table, it is assumed that the first qubit represents the control qubit in the CNOT and Fredkin gates. The Toffoli operation flips the target qubit conditional on two other qubits being 1. It is assumed in this table that the Toffoli is conditional upon the first two qubits being 1.

FIGURE CAPTIONS

Fig. 1. A quantum circuit that implements the boosting procedure. The qubits are represented by horizontal lines and their states are transformed by circuit elements representing unitary operations. The \oplus symbol indicates a bit flip. The \bullet symbol denotes a control qubit — the operation it controls is performed if and only if the control qubit is in the state $|1\rangle$. The controlled-swap operation has been replaced by an equivalent set of gates: two CNOT's and a Toffoli (Table 1).

Fig. 2. Pulse sequence to implement the boosting procedure. X , Y , and Z represent 90° rotations about those respective axes. \bar{X} represents a negative 90° rotation, X^2 denotes a 180° rotation and $X^{1/2}$ denotes a 45° rotation. This pulse sequence is designed for molecules with $J_{ab} < 0$ and $J_{ac}, J_{bc} > 0$.

Fig. 3. Experimentally measured spectra of spin a (Left), spin b (Center) and spin c (Right), after a readout pulse on the corresponding spin, for the spin system in thermal equilibrium (Top) and after applying the boosting procedure (Bottom). The real part of the spectra is shown, and the spectra were rescaled in order to obtain unit amplitude for the thermal equilibrium spectra. Frequencies are in Hz with respect to the Larmour frequency of the respective spins.

Fig. 4. Pictorial representation of the theoretical (left) and experimentally measured (right) density matrices, shown in magnitude with the sign of the real part (all imaginary components were very small).

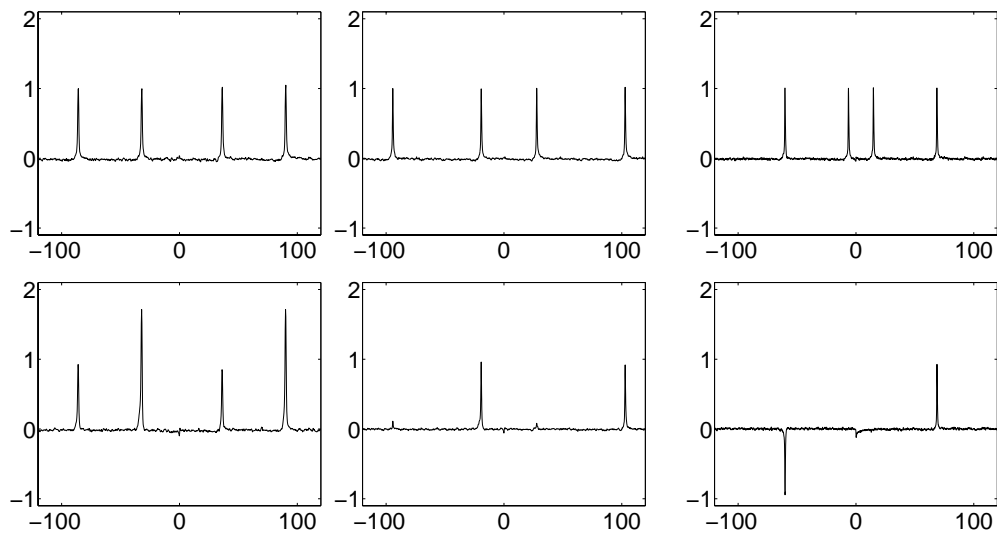


Figure 3

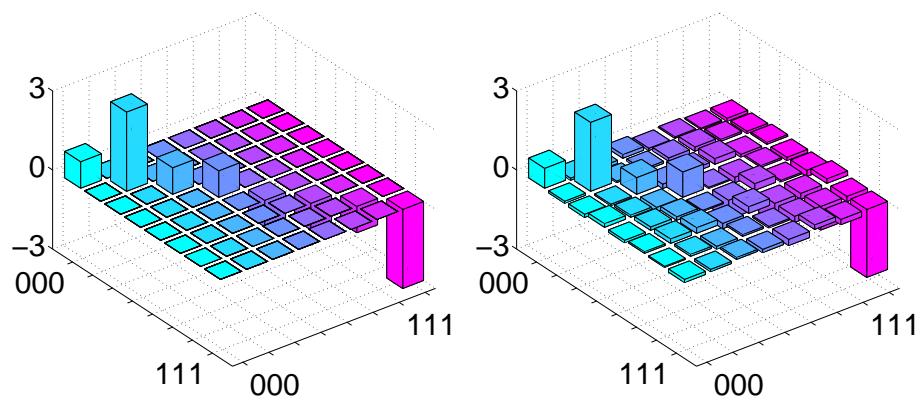


Figure 4