Experimental realization of a highly structured search algorithm

Xiwen Zhu, Ximing Fang, Mang Feng, Fei Du, Kelin Gao and Xi’an Mao

Laboratory of Magnetic Resonance and Atomic and Molecular Physics,
Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences,
Wuhan 430071, P. R. China

(March 31, 2022)

Abstract

The highly structured search algorithm proposed by Hogg[Phys.Rev.Lett. 80,2473(1998)] is implemented experimentally for the 1-SAT problem in a single search step by using nuclear magnetic resonance technique with two-qubit sample. It is the first demonstration of the Hogg’s algorithm, and can be readily extended to solving 1-SAT problem for more qubits in one step if the appropriate samples possessing more qubits are experimentally feasible.

PACS numbers: 89.70.+c, 03.65.-w, 02.70.-c
Quantum computers[1-5] can outperform classical ones owing to utilization of quantum mechanical effects. The potential for quantum parallel computing mainly resulted from superpositions and entanglements of quantum states has made quantum computers capable of solving classically intractable problems (such as factoring large integers[3]) and finding tractable solutions more rapidly(e. g., searching an unsorted database[6]). However, carrying out an actual quantum computing is much difficult although the rudiment of the quantum computing is easily understood and several quantum algorithm have been discovered. Among the approaches meeting the requirement for performing quantum computing, the nuclear magnetic resonance(NMR) technique[7,8] is considered to be one of current promising method, with which the Deutsch-Jozsa algorithm[9] and Grover’s search one[6] has been experimentally implemented with two-qubit samples[10-13]. Recently, it was reported that an algorithmic benchmark has been experimentally realized using NMR with seven qubits[14]. It was easily found from those works that NMR can act as a considerably satisfactory small-scaled quantum computer to test the simple cases of the various quantum algorithm. In this contribution, also using NMR scheme with two-qubit sample, we report the first experimental demonstration of another quantum search algorithm. This algorithm, called a highly structured quantum search algorithm[15], was claimed to be much more efficient than Grover’s algorithm[6] that ignores the problem structure, and can be exploited in many practical examples instead of for academic study alone as an artificial problem[9].

The Hogg’s algorithm is associated with the combinatorial searching known as nondeterministic polynomial-time problems(NP)[16], an important class of intractable problems. Its prototype is the satisfiability problems(SAT)[16]. A SAT consists of a logic formula in $n$ boolean variables, $V_1,...,V_n$, and the requirement to find an assignment, specifying a value for each binary variable, that makes the formula true. The logic formula can be expressed as a conjunction of $m$ clauses and each clauses is a disjunction of some variables. When all the clauses have exactly $k$ variables, the problem is called k-SAT, with 1-SAT being the simplest case. Combinatorial search aims at seeking the solution of a SAT from the total of $2^n$ assignments. In general, the computational cost of solving a SAT grows exponentially
with \( n \) in the worst case, making the SAT one of the most difficult NP problems [16]. For a few simple cases like 1-SAT and 2-SAT, however, solutions can be quickly and accurately determined without exponential cost using the regular structure of the problem. As each false clause for a given assignment is counted as a conflict, solutions are assignments with no conflicts. The classical search cost for such cases is \( O(n) \) due to each clause eliminating one value for a single variable, but the quantum counterpart with Hogg’s algorithm for 1-SAT and maximally constrained k-SAT a single step [15], with the help of quantum parallelism and interference combined with the problem structure, which shows very high efficiency for large \( n \).

Actually, Hogg’s algorithm consists of three stages [15]. First, one makes an equal superposition of bases, \( |s> \), of the \( n \) two-state quantum system as the initial state \( |\psi_i> = 2^{-\frac{n}{2}} \sum_s |s> \), with bit strings \( s \) being all \( 2^n \) assignments of \( n \) variables. Secondly, a transformation \( R \) is applied on \( |\psi_i> \). The elements \( R_{ss} \) of the diagonal matrix \( R \) are determined by the conflicts \( c_s \) of \( s \), which are governed by the constraints expressed in clauses of the logic formula. It is explicitly expressed as

\[
R(s) = \begin{cases} 
\sqrt{2} \cos \left( \frac{2c - 1}{4} \right) & \text{for even } m \\
i^c & \text{for odd } m.
\end{cases}
\]  

Finally, an operation \( U \) with the form

\[
U_{rs} = \begin{cases} 
2^{-\frac{n-1}{2}} \cos \left[ \left( n - m + 1 - 2d \right) \frac{\pi}{4} \right] & \text{for even } m \\
2^{-\frac{n}{2}} e^{i(n-m)\frac{\pi}{4}} (-i)^d & \text{for odd } m,
\end{cases}
\]

is acted. It can be seen that the matrix elements \( U_{rs} \) depend only on the Hamming distance \( d_{r,s} \) between \( r \) and \( s \). As it describes the inconsistency of all the corresponding bits of bit strings \( r \) and \( s \), \( d_{r,s} \) has some correlation with conflicts \( c_s \). By exploiting the intrinsic relation between \( d_{r,s} \) and \( c_s \) and ingeniously constructing \( R_{ss} \) and \( U_{rs} \) with \( d_{r,s} \) and \( c_s \), making the combined transformation \( UR \) on \( |\psi_i> \) once is able to find the expected state, i. e., \( UR |\psi_i> = |\psi_0> \), which has equal amplitudes among solutions and no amplitudes among nonsolutions.
In the view of quantum physics, Hogg’s algorithm subtly makes use of the properties of quantum superposition and interference. When the calculating system is prepared on the equal superposition state, $|\psi_i\rangle = 2^{-\frac{n}{2}} \sum_s |s\rangle$, all the possible values, which can be assigned to the logical formula, regardless correct or incorrect, are embodied in the state. Then the state is subjected to the transform $R$, which gives a varied phase to each component state of the superposition state according to its conflicts $c_s$. The final operation $U$ destructively annihilates every component state that its conflict is not zero, constructively enhances the correct component state that its conflicts is zero, finds out the exact component state that satisfies the logical formula. In one word, the essence of searching achieved in a single step is to examine all the assignments simultaneously and to make use of quantum interference embedded in UR. By a single step we mean the number of search steps or sequentially examined assignments, not the number of elementary computational operations required.

Our implementation of Hogg’s algorithm was performed using solution NMR, applied to an ensemble of carbon-13 labelled chloroform molecules ($^{13}$CHCl$_3$). Two heteronuclear spins $^1$H and $^{13}$C in $^{13}$CHCl$_3$ work as two qubits in our quantum computing. Similar to other experiments[9-12,14,17-19] of quantum information processing using NMR, all the logic operations were realized by a specified sequence of radio-frequency (RF) pulses and the spin-spin coupling between the nuclei, and should be finished in the period of time much shorter than the relaxation times $T_1$ and $T_2$ of the nuclei in order to minimize the decoherence effect.

A quantum circuit for achieving this highly structured search in a two-qubit system is shown in Fig. 1. The algorithm starts in the state $|\psi_s\rangle = |00\rangle$, labelling the states of $^1$H and $^{13}$C spins from left to right respectively. As the state of a bulk sample at room temperature is described by a density matrix $\rho_{th}$ for a thermally equilibrated system, we prepared an effective pure state $\rho = |00\rangle\langle 00|$ by temporal averaging[20], with which a deviation density matrix with diagonal elements of $\text{diag}(\rho_s) = [1,0,0,0]$ could be extracted from the summation over cyclic permutations of the populations of the $|01\rangle$, $|10\rangle$, and $|11\rangle$ states three times on the thermal matrix $\rho_{th}$. The Hadamard gates $H$ in Fig. 1 were
implemented by using RF pulse sequence \( \left( \frac{\pi}{2} \right)_y (\pi)_x \) or its equivalents and thus a uniform superposition state denoted by the density matrix \( \rho_i = |\psi_i><\psi_i| \) with \( \text{diag}(\rho_i)=[1,1,1,1] \) was obtained. Then two crucial operations R and U were applied, which are related to the problem structure and expressions for the logic formula and lead to the enhancement of solution states and the cancel of nonsolution states.

For our two-qubit system (i.e., \( n=2 \)), \( m \), the number of clauses in the 1-SAT formula with satisfiable solutions can be assumed 2 or 1. When \( m = 3 \) and 4, no satisfying assignment exists due to over-constrained formula being unsatisfiable. Four satisfiable formulas in the \( m = 2 \) case are \( V_1 \land V_2, V_1 \land \overline{V}_2, \overline{V}_1 \land V_2 \) and \( \overline{V}_1 \land \overline{V}_2 \), where \( \overline{V}_i \) \( (i = 1, 2) \) are the negation of \( V_i \). The corresponding solutions are easily found to be \( |11>, |10>, |01> \) and \( |00> \) respectively, where the logic variable with subscript 1 corresponds to the high qubit and 2 the low qubit. Similarly, the formulas for \( m=1 \) are \( V_2, V_1, \overline{V}_2 \) and \( \overline{V}_1 \), corresponding to the unnormalized answer states \( |01 > + |11 >, |10 > + |11 >, |00 > + |01 > \) and \( |00 > + |01 > \), respectively. According to the number of states in the solutions, they can be called as single- and multiple- item searching. The algorithm on two instances of 1-SAT was experimentally demonstrated: one for \( m = 2 \) with clauses \( V_1 \) and \( V_2 \), and the other for \( m = 1 \) with clause \( V_2 \).

First of all, we have to derived the expressions for R and U from Ref.[15]. With Eq.(1), after calculating the conflicts \( c \) of each string assigned to the logical formula respectively, the elements of the diagonal matrices \( R_{V_1 \land V_2} \) and \( R_{V_2} \) were calculated to be \( \text{diag}(R_{V_1 \land V_2}) = [-1, 1, 1, 1] \) and \( \text{diag}(R_{V_2}) = [i, 1, i, 1] \). U could be represented by \( WTW \), where \( W = H_1 \otimes H_2 \) with \( H_i \) being the Hadamard gates, and \( \Gamma \) is a diagonal matrix with the diagonal elements

\[
\Gamma_{rr} = \begin{cases} 
\sqrt{2} \cos \left[(m-2|r| - 1)\frac{\pi}{4}\right] & \text{for even } m \\
|^{r|}e^{-i m \frac{\pi}{4}} & \text{for odd } m.
\end{cases}
\]

Elements of the diagonal matrices \( \Gamma \) for \( m = 2 \) and \( m = 1 \) were evaluated respectively as \( \text{diag}(\Gamma_{m=2}) = [1, 1, 1, -1] \) and \( \text{diag}(\Gamma_{m=1}) = [1, i, i, -1] \).

In order to realize the transformations with NMR, we designed the following RF pulse
sequences respectively:

\[ R_{V_1 \land V_2}: \left( \frac{\pi}{2} \right)_{y_1} \left( \frac{\pi}{2} \right)_{x_1} \left( \frac{\pi}{2} \right)_{\pm y_1} - \frac{1}{2} \left( \frac{\pi}{2} \right)_{y_2} \left( \frac{\pi}{2} \right)_{x_2} \left( \frac{\pi}{2} \right)_{\pm y_2} \]

\[ R_{V_2}: \left( \frac{\pi}{2} \right)_{y_1} \left( \frac{\pi}{2} \right)_{x_1} \left( \frac{\pi}{2} \right)_{\pm y_1} \]

\[ \Gamma_{m=2}: \left( \frac{\pi}{2} \right)_{y_1} \left( \frac{\pi}{2} \right)_{\pm x_1} \left( \frac{\pi}{2} \right)_{\pm y_1} - \frac{1}{2} \left( \frac{\pi}{2} \right)_{y_2} \left( \frac{\pi}{2} \right)_{\pm x_2} \left( \frac{\pi}{2} \right)_{\pm y_2} \]

\[ \Gamma_{m=1}: \left( \frac{\pi}{2} \right)_{y_1} \left( \frac{\pi}{2} \right)_{x_1} \left( \frac{\pi}{2} \right)_{y_1} \left( \frac{\pi}{2} \right)_{y_2} \left( \frac{\pi}{2} \right)_{x_2} \left( \frac{\pi}{2} \right)_{\pm y_2} \]

To make the best use of the available coherence time and to diminish errors due to the increased number of RF pulses, we finally optimized or reduced the pulse sequence constructed from the executing pulses of H, Γ and R mentioned above with the help of NMR principle[21]. The reduced pulse sequence for (UR)\(_V\) shown in Fig. 2 were applied upon \(\rho_i\), resulting the output matrix \(\rho_0 \equiv |\psi_0 \rangle \langle \psi_0| = (UR)\rho_i(UR)^\dagger\).

In order to read out the results of Hogg’s algorithm accurately, a method of quantum state tomography[22] was adopted to reconstruct all the elements of the output density matrix \(\rho_0\). For this end, we applied different read-out pulses immediately after the searching pulses UR, one for each run. Explicitly, nine pulses \(E_1 E_2\), \(E_1 \left( \frac{\pi}{2} \right)_{x_2}\), \(E_1 \left( \frac{\pi}{2} \right)_{y_2}\), \(\left( \frac{\pi}{2} \right)_{x_1} E_2\), \(\left( \frac{\pi}{2} \right)_{x_1} \left( \frac{\pi}{2} \right)_{x_2}\), \(\left( \frac{\pi}{2} \right)_{x_1} \left( \frac{\pi}{2} \right)_{y_2}\), \(\left( \frac{\pi}{2} \right)_{y_1} E_2\), \(\left( \frac{\pi}{2} \right)_{y_1} \left( \frac{\pi}{2} \right)_{x_2}\) and \(\left( \frac{\pi}{2} \right)_{y_1} \left( \frac{\pi}{2} \right)_{y_2}\) were exploited, where \(E_i (i = 1, 2)\) means no pulse acted on the i-th spin. Then we calculated the signal intensities by integrating the proton and carbon spectral lines acquired in each run and reproduced the whole matrix \(\rho_0\) using the least-square fitting to the coupled equations connecting the signal intensities with the matrix elements. The recovered matrices \(\rho_0\) from the experimental data were depicted in Fig. 3, along with the theoretical ones for comparison. It is clearly seen from Fig. 3 that only the elements of \(<11|\rho_0(V_1 \land V_2)|11\rangle\), \(<01|\rho_0(V_2)|01\rangle\), \(<01|\rho_0(V_2)|11\rangle\), \(<11|\rho_0(V_2)|01\rangle\) and \(<11|\rho_0(V_2)|11\rangle\) are significant, which justifies the searched items to be \(|11\rangle\) for \(V_1 \land V_2\) and unnormalized \(|01\rangle + |11\rangle\) for \(V_2\) formula. Due to experimental errors, however, several elements that should be zero theoretically still have small amounts of modulus, with the maxima being 8% for single-item and 19% for multiple-item searching.

Errors in the experiments result from several sources. The effective pure state \(|00\rangle\) prepared by temporal averaging is generally not ideal, and small residual populations in the states \(|01\rangle\), \(|10\rangle\) and \(|11\rangle\) of the deviation density matrix will surely cause errors in the
later stage of experiments. The inhomogeneity of RF fields and static magnetic fields and
imperfections of the pulse-length calibration are also important sources of errors. Although
we have tried to minimize these effects by careful adjustments of and measurements with the
apparatus, some factors were still not well under control. Lastly but not insignificantly, losses
of the coherence and populations of the density matrices in the whole process of experiments
will lead to deviations of measured data from those expected by theory, especially for the off-
diagonal elements. Perhaps that is why the maximum error in the multiple-item searching
is larger than that in the single-item case. In all senses, minimizing experimental errors in
all available ways is essential to accurately operating NMR quantum computers.

We have experimentally demonstrated a quantum algorithm for the highly structured
combinatorial searching and found solutions to the 1-SAT problem in one algorithmic step
almost surely using an NMR quantum computer with 2 qubits. By contrasting with other
search methods that ignore the problem structure requiring $O(2^n)$ steps classically and
$O(2^{\frac{n}{2}})$ steps on quantum computers[6], the searching with Hogg’s algorithm can be accomplished
in principle more efficiently. However, there is no difference between Hogg’s algorithm and
Grover’s one when only two qubits are considered. The potential of the high efficiency owned
by Hogg’s algorithm will be displayed in solving various 1-SAT problems for $n > 2$ qubits
in one step with current NMR technique, which can be readily extended from the present
experiment, if the appropriate samples possessing more qubits can be experimentally feasible.
Furthermore, Hogg’s algorithm for 1-SAT could be generalized to the maximally constrained
k-SAT problems[15], which have practical examples such as scheduling, finding low energy
states of spin glasses and proteins, and automatic theorem proving. While scaling up an
NMR computer to much large systems poses daunting challenges, building such a device
with a few qubits by some creative approaches for demonstrating algorithms stated above
and the others is promising.

We thank Xijia Miao for help in the early stage of experiments. This work was supported
by the Chinese Academy of Sciences and National Natural Science Foundation of China.
REFERENCES

[1] R.P.Feynman, Simulating physics with computers. Int.J.Theor.Phys. 21 (1982)467-488.

[2] D.Deutsch, Quantum theory, the Church-Turing principle and the universal quantum computer. Proc. Soc. Lond. A400(1985)97-117.

[3] P.Shor, Algorithms for quantum computation:discrete logarithms and factoring. Proc. 35th Annu. Symp. on Found. of Computer Science, (IEEE Comp. Soc. Press, Los Alomitos, CA,1994)124-134.

[4] D.P.DiVincenzo, Quantum computation. Science 270(1995)255-261.

[5] S.Lloyd, Quantum-mechanical computers. Sci. Am. 273(1995)44-50.

[6] L.K.Grover, Quantum mechanics helps in searching for a needle in a haystack. Phys. Rev. Lett. 79(1997)325-328.

[7] D.G.Cory, A.F.Fahmy and T.F.Havel, Ensemble quantum computing by NMR spectroscopy. Proc. Nat. Acad. Sci. USA 94(1997)1634-1639.

[8] N.Gershenfeld, I.L.Chuang, Bulk spin resonance quantum computation. Science 275(1997)350-356.

[9] D.Deutsch and R.Jozsa, Rapid solution of problems by quantum computation. Proc. R. Soc. Lond. A 439(1992)553-558.

[10] I.L.Chuang, N.Gershenfeld, and M.Kubinec, Experimental implementation of fast quantum searching. Phys. Rev. Lett. 80(1998)3408-3411.

[11] J.A.Jones, M.Mosca, and R.H.Hansen, Implementation of a quantum search algorithm on a nuclear magnetic resonance quantum computer. Nature 393(1998)344-346.

[12] I.J.Chuang, L.M.K.Vandersypen, X.L.Zhou, D.W.Leung, and S.Lloyd, Experimental realization of a quantum algorithm. Nature 393(1998)143-146.
[13] J.A.Jones and M.Mosca, Implementation of a quantum algorithm on a nuclear magnetic quantum computer. J. Chem. Phys. 109 (1998)1648-1653.

[14] E.knill, R.Laflamme, R.Martinez and C.H.Tseng, An algorithmic benchmark for quantum information processing, Nature, 404(2000)368-370.

[15] T.Hogg, Highly structured searches with quantum computers. Phys. Rev. Lett. 80(1998)2473-2476.

[16] M.R.Garey and D.S.Johnson, Computers and Intractability: a Guide to the Theory of NP-Completeness (Freeman, San Francisco, 1979).

[17] R.Laflamme, E.Knill, W.H.Zurek, P.Catasti and S.V.S.Mariappan, Greenberg-Horne-Zeilinger states. Phil. Trans. R. Soc. Lond. A 356(1998)1941-1947.

[18] D.G.Cory, M.D.Price, W.Maas, E.Knill, R.Laflamme, W.H.Zurek, T.F.Havel and S.S.Somaroo, Experimental quantum error correction. Phys. Rev. Lett. 81(1998)2152-2155.

[19] M.A.Nielsen, E.Knill and R.Laflamme, Complete quantum teleportation using nuclear magnetic resonance. Nature 396(1998)52-55.

[20] E.Knill, I.L.Chuang and R.Laflamme, Effective pure states for bulk quantum computation. Phys. Rev. A 57(1998)3348-3363.

[21] R.Ernst, G.Bodenhausen and A.Wokaun, Principles of Nuclear Magnetic Resonance in One and Two Dimensions(Oxford Univ. Press,Oxford,1990).

[22] I.L.Chuang, N.Gershental, M.Kuhinec and D.Leung, Bulk quantum computation with nuclear magnetic resonance: theory and experiment. Proc. R. Soc. Lond. A 454(1998)447-467.
Captions of the figures

Figure 1  A quantum circuit for implementing a highly structure search algorithm on a two-qubit computer. Two Hadamard gates $H \otimes H$ transform an effective pure states $|\psi_s> = |00>$ into a uniform superposition state $|\psi_i>$, which is then transformed to the answer state $|\psi_0>$ after the action of gates $R$ and $U$. For the definition of $R$ and $U$, see text.

Figure 2  The reduced NMR pulse sequences used to execute a) $(UR)_{V_1 \land V_2}$ and b) $(UR)_{V_2}$ operations. Narrow and wide boxes correspond to $\frac{\pi}{2}$ and $\pi$ pulses respectively. $X$ and $Y$ denote the pulses along the x- and y-axis, $\overline{X}$ and $\overline{Y}$, opposite to the x- and y-axis. The time period $\tau$ is set equal to $\frac{1}{4J}$, where $J$ is the size of the spin-spin coupling between nuclei $^1H$ and $^{13}C$. Experiments were performed using a Bruker ARX500 spectrometer. $^{13}C$-labelled CHCl$_3$ were obtained from Cambridge Isotope Laboratories.

Figure 3  Experimentally recovered and theoretically expected deviation density matrices, $\rho_0$, after completion of the combinatorial search with the aim of satisfying logic formulas of both $V_1 \land V_2$ and $V_2$. The ordinate represents the modulus of matrix elements of $\rho_0$ (not normalized). The numbers 0, 1, 2 and 3 in the horizontal plane denote the subscripts $|00>$, $|01>$, $|10>$ and $|11>$ of the elements, respectively. a) Experiment for $V_1 \land V_2$, b) Theory for $V_1 \land V_2$, c) Experiment for $V_2$ and d) Theory for $V_2$. 
Fig. 1
