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# Quantum demonstration of a bio-molecular solution of the satisfiability problem on spin-based ensemble*

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DNA computation (DNAC) has been proposed to solve the satisfiability (SAT) problem due to operations in parallel on extremely large numbers of strands. This paper attempts to treat the DNA-based bio-molecular solution for the SAT problem from the quantum mechanical perspective with a purpose to explore the relationship between DNAC and quantum computation (QC). To achieve this goal, it first builds up the correspondence of operations between QC and DNAC. Then it gives an example for the case of two variables and three clauses for details of this theory. It also demonstrates a three-qubit experiment for solving the simplest SAT problem with a single variable on a liquid-state nuclear magnetic resonance ensemble to verify this theory. Some discussions are made for the potential application and for further exploration of the present work.

**Keywords:** DNA computation, liquid-state nuclear magnetic resonance, SAT problem, quantum computation

**PACC:** 0367, 8760I, 8700

In recent years there have been many outstanding breakthroughs in the molecular/DNA computation (DNAC) proposed by Feynman in 1961,[1] among which the famous satisfiability (SAT) problem has been paid a lot of attention by the methods with DNA strands[2−4] due to the potentially vast parallelism of DNAC.

On the other hand, quantum computation (QC), another proposal by Feynman,[5] has drawn considerable attention over the past decades. Eight atomic qubits[6] and six photonic qubits[7] have been entangled so far, respectively, and simple quantum algorithms have been tested experimentally.[8] Within the QC framework, the type of unstructured problems, such as SAT, can be in principle figured out in finite size by the Grover search algorithm,[9] which has a square root speedup in comparison with classical methods for finding the answer.

A natural question arises: as both the DNAC and QC employ parallelism in reduction of computational complexity, is there any relationship between them? To answer this question, we are trying to conduct an investigation in the present paper to carry out a DNA-based bio-molecular solution quantum mechanically for the SAT problem. We will first present a brief review for the basic operations in DNAC and in QC, for which we could set up some correspondence. Then we will try to carry out a DNAC quantum mechanically by using an example of SAT with two variables and three clauses. To check our theory, we will also experimentally solve a simplest SAT problem with only one variable and one clause, i.e., $F = (u_1)$, by the spin-based liquid-state NMR ensemble. Some discussions regarding the present work would be made.

Generally speaking, the basic DNAC operations[10] involved in the bio-molecular solution are Append, Extract, Discard, Amplify, Merge, Detect and Read. The operation Append, including Append–Head and Append–Tail, is to put a short DNA strand to the head and to the tail of a long

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strand, respectively. That is to say, Append–Head $(B, u_j) = \{u_j, B_n, B_{n-1}, \ldots, B_2, B_1\}$, and Append–Tail $(B, u_j) = \{B_n, B_{n-1}, \ldots, B_2, B_1, u_j\}$ , with $B$ a set consisting of a number of elements $B_k$ $(k = 1, \ldots, n)$. Extract is to extract some of the required DNA strands. In most operations, Extract results in a separation of one tube into two with one tube involving the required strands and the other involving the rest. The corresponding formulas are $+\{U, u_j^1\} = \{u_n, u_{n-1}, \ldots, u_j^1, \ldots, u_2, u_1\}$ and $-\{U, u_j^1\} = \{u_n, u_{n-1}, \ldots, u_j^0, \ldots, u_2, u_1\}$ with $U$ the set involving elements $u_k$ $(k = 1, \ldots, n)$ and $u_j^1$ and $u_j^0$ denoting values of $u_j$ to be 1 and 0, respectively. Discard is to null a tube, i.e., removing each DNA strand from the tube. Amplify replicates all of the DNA strands in the test tube, which creates a number of identical copies and then discard the original one by Discard. Merge corresponds to the operation to pour many tubes of DNA strands into one tube without any change in the individual strands, which could be described by $\cup P_1 \cup P_2 \cup \ldots \cup P_n$, with $P_k$ $(k = 1, 2, \ldots, n)$ being a tube with DNA stands. Detect leads to a result 'YES' once there is at least one DNA strand in the tube, or to 'NO' otherwise. Read gives an explicit description of one DNA strand, no matter how many molecules in the tube.

On the side of QC, there are some basic operations constituting universal QC, where the most frequently mentioned gates are $R(\theta) = \begin{pmatrix} 1 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\,\theta} \end{pmatrix}$ for the qubit encoding $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, a Hadamard gate $H = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}/\sqrt{2}$ to change $|0\rangle$ to $(|0\rangle + |1\rangle)/\sqrt{2}$ and $|1\rangle$ to $(|0\rangle - |1\rangle)/\sqrt{2}$, and a controlled-NOT gate $\mathrm{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$. To be more efficient, we sometimes employ three-qubit Toffoli gate TOFF to flip the target qubit when the two control qubits are both in state $|1\rangle$.

Comparing QC with DNAC, we could find some relations between them. Quantum mechanically, *Append* could be described as a tensor product, i.e., Append–Head $(B, u_j) = \{u_j\} \otimes \{B\}$ and Append–Tail $(B, u_j) = \{B\} \otimes \{u_j\}$, where $\{u_j\}$ and $\{B\}$ are denoted by matrices. The operation Extract could be carried out by CNOT, which leads $(|0\rangle + |1\rangle)|0\rangle/\sqrt{2}$ to $(|0\rangle|0\rangle + |1\rangle|1\rangle)/\sqrt{2}$ , where the control qubit is the one we hope to remain and the target qubit storing the result of execution is the ancilla. After a measurement is made on the target qubit, the control qubit will be left in $|1\rangle$ or $|0\rangle$, corresponding to the action of $+\{U, u_j^1\}$ and $-\{U, u_j^1\}$ in DNAC. On the other hand, the Hadamard gate in QC could be carried out by the operations of DNAC with Extract to separate two subsets respectively including $|0\rangle$ and $|1\rangle$, and then with Append and Merge to realize $|0\rangle \to (|0\rangle + |1\rangle)/\sqrt{2}$ and $|1\rangle \to (|0\rangle - |1\rangle)/\sqrt{2}$. To be specific, we give an example below to simulate quantum superposition by operations in DNAC. We initially have an empty set $\{\phi\}$, and replicate it by Amplify$\{\phi\}$ to be two empty sets. Append–Tail$\{\phi, |0\rangle\}$ and Append–Tail$\{\phi, |1\rangle\}$ yield the sets $\{|0\rangle\}$ and $\{|1\rangle\}$, respectively. After the operation Merge, we could have a superposition in the set $\{|0\rangle + |1\rangle\}$, equivalent to $H|0\rangle$ in QC. Repeating the above steps, i.e., with Amplify, then Append–Tail, and Merge, we could get the set $\{(|0\rangle + |1\rangle)|0\rangle + (|0\rangle + |1\rangle)|1\rangle\}$, actually corresponding to $H|0\rangle \otimes H|0\rangle$ in QC. Nevertheless, it seems that DNAC could not fully accomplish the jobs by QC. For example, the QC operation $R(\theta)$ with $0 < \theta < 2\pi$ could not be efficiently simulated by DNAC. On the contrary, quantum computation could carry out any job by DNAC in a more efficient way.

In what follows, we will solve a SAT problem quantum mechanically following the route in DNAC. Consider a case as an example with the formula

$$F = (u_2 \vee u_1) \wedge (\overline{u}_2 \vee \overline{u}_1) \wedge (u_1), \tag{1}$$

where $u_2$ and $u_1$ are Boolean variables whose values can be 0 (false) or 1 (true). $\vee$ is the "logical OR" operation with $u_2 \vee u_1 = 0$ only if $u_2 = u_1 = 0$, and $\wedge$ is the "logical AND" operation with $u_2 \wedge u_1 = 1$ only if $u_2 = u_1 = 1$. $\overline{u}_2$ and $\overline{u}_1$ are the operations "NEGATION" of $u_2$ and $u_1$, respectively, i.e., $\overline{u}_2$ being 0 if $u_2 = 1$ and being 1 if $u_2 = 0$. The SAT problem is to find appropriate values for $u_2$ and $u_1$ to make the formula $F$ true.

The DNA-based bio-molecular solution for the above problem could be found in detail in Ref.[2]. We will instead present our solution steps based on its quantum mechanical correspondence. We first employ

superposition states by the Hadamard gate on each qubit to accomplish the PREPARATION in DNAC. Then we use CNOT, along with auxiliary qubits, to replace Extract, and the logic AND and OR could be carried out by quantum circuits,[11] as shown in Fig.1.

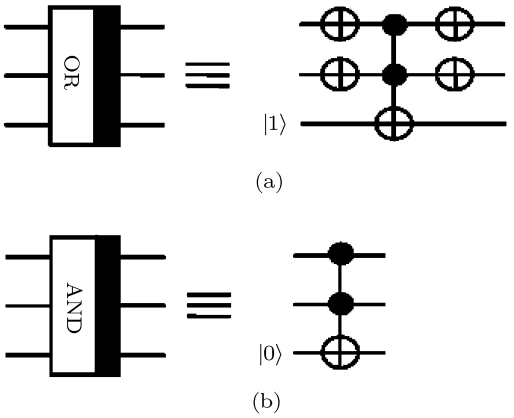



**Fig.1.** Quantum circuits for (a) the operation AND, i.e., a three-qubit TOFF gate, and (b) the operation OR with a three-qubit TOFF gate sandwiched by four NOT gates, where the dark bar side means the output side.

To solve Eq.(1), we have to employ four quantum registers $|u_2u_1\rangle$, $|y_2y_1\rangle$, $|r_2r_1r_0\rangle$ and $|c_3c_2c_1c_0\rangle$, as shown in Fig.2, where $|u_2\rangle$ and $|u_1\rangle$ are qubits corresponding to the variables $u_2$ and $u_1$ in Eq.(1) and we initially set them to be zero.

The qubits $|y_2\rangle$ and $|y_1\rangle$, also initially being zero, are auxiliary qubits storing the results of CNOT, respectively. The third register stores the results of OR, where the qubits inside are initially prepared to be $|r_2^1\rangle$, $|r_1^1\rangle$, and $|r_0^1\rangle$, with the superscripts being values of the qubits. As logic OR between two variables is made by three qubits (see Fig.1), we need three qubits in this register and their initial values are set by the requirement for logic OR. After each time with the data transferred to the third register from the second one, $|y_2\rangle$ and $|y_1\rangle$ will be nulled for later use. The fourth register, including four qubits, are used for storing the results of AND, where except $|c_0^1\rangle$, other qubits are initially zero.

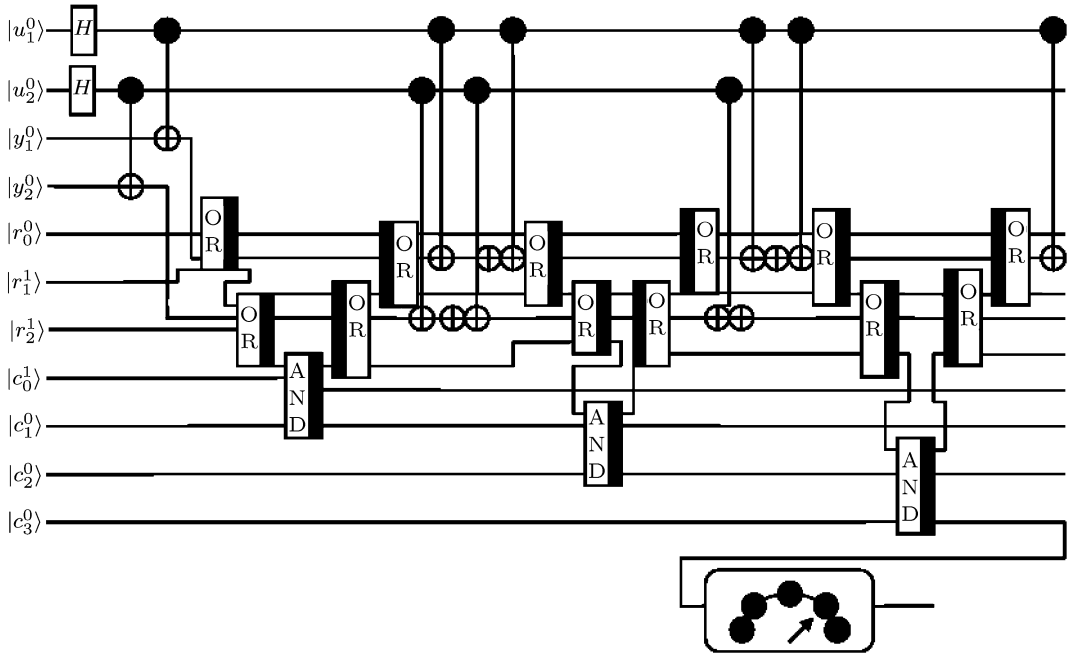



**Fig.2.** Quantum circuits with eleven qubits for solving a three-clause SAT problem with two variables, where some of the registers hold qubits and some for auxiliary qubits, as explained in the text. The superscript 0 or 1 means the initial value of the qubit. The block with the dark bar on the left side, used to restore the register, means a reverse operation of the corresponding block with the dark bar on the right. CNOT corresponds to the DNAC operation Extract $+\{U, u_j^1\}$ and $-\{U, u_j^1\}$, and NOT plus CNOT takes into account $+\{U, u_j^0\}$ and $-\{U, u_j^0\}$ in DNAC.

The involvement of four qubits is due to the three clauses and the requirement for making logic AND. After each AND operation, the results are stored in $|c_3\rangle$, $|c_2\rangle$ or $|c_1\rangle$, respectively, and we have to restore the qubits in the third register to be $|r_2^1\rangle$, $|r_1^1\rangle$ and $|r_0^0\rangle$ for later use repeatedly. Based on the operation

correspondence mentioned above, we will design a quantum circuit following the computational route in DNA, where the qubits are input from the left-hand side of the circuit. Following the gates in Fig.2 step by step, we may straightforwardly obtain the state

$$\begin{aligned}&1/2 * (|c_3^0\rangle|c_2^0\rangle|c_1^0\rangle|c_0^1\rangle|r_2^1\rangle|r_1^1\rangle|r_0^0\rangle|y_2^1\rangle|y_1^0\rangle|u_2^0u_1^0\rangle + |c_3^0\rangle|c_2^1\rangle|c_1^1\rangle|c_0^1\rangle\\&|r_2^1\rangle|r_1^1\rangle|r_0^0\rangle|y_2^0\rangle|y_1^0\rangle|u_2^1u_1^0\rangle + |c_3^1\rangle|c_2^1\rangle|c_1^1\rangle|c_0^1\rangle|r_2^1\rangle|r_1^1\rangle|r_0^0\rangle|y_2^0\rangle|y_1^0\rangle|u_2^0u_1^1\rangle\\&+ |c_3^0\rangle|c_2^0\rangle|c_1^1\rangle|c_0^1\rangle|r_2^1\rangle|r_1^1\rangle|r_0^0\rangle|y_2^0\rangle|y_1^0\rangle|u_2^1u_1^1\rangle),\end{aligned} \tag{2}$$

where the solution is the state regarding $|c_3^1\rangle$. So once we have measured $|c_3^1\rangle$, the state in expression (2) collapses to $|c_2^1\rangle|c_1^1\rangle|c_0^1\rangle|r_2^1\rangle|r_1^1\rangle|r_0^0\rangle|y_2^0\rangle|y_1^0\rangle|u_2^0u_1^1\rangle$, which implies the solution of the SAT in Eq.(1) to be $u_1 = 1$ and $u_2 = 0$. Of course this measurement succeeds with the probability of 1/4. We will return to this point later.

We have experimentally solved a simplest SAT case involving a single variable and a single clause, i.e., $F = (u_1)$, by nuclear magnetic resonance (NMR) techniques based on the DNAC and QC correspondence. The NMR approach has been widely employed for quantum information processing over the past several years due to its mature and well-controllable technology.[12] Although the quantum information processing by NMR is made on ensembles of nuclear spins, instead of individual spins, NMR techniques have remained to be the most convenient experimental tool to demonstrate quantum information processing.[13−15]

As shown in Fig.3, there are three qubits involved, among which $|u_1\rangle$ is the qubit holding the variable, $|y_1\rangle$ is the ancilla of $|u_1\rangle$, and $|c_1\rangle$ is to store the evaluating result. The last CNOT is to restore the qubit $|y_1\rangle$.

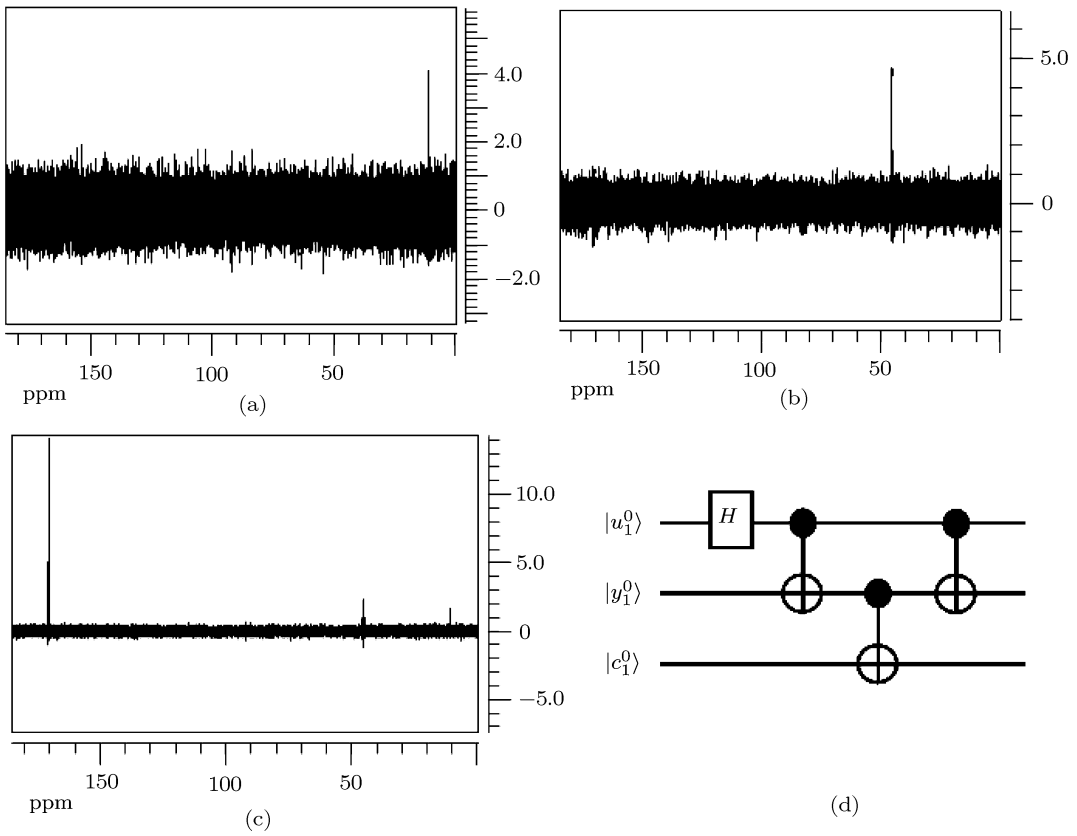



**Fig.3.** NMR experimental spectra for qubit outputs of solution to $F = (u_1)$ and the quantum circuit for solving $F = (u_1)$, where the plots from the top left, top right to the bottom left correspond to (a), (b) and (c) for the outputs regarding the first, second and third qubits, respectively. The measurement should be made on the third (i.e., the bottom) qubit of the quantum circuit. But due to the unique feature of NMR, we need additional gates in our experiment for the readout of each qubit, which are described in the text, but omitted here.

We employ NMR techniques[16] to prove the validity of the constructed quantum circuit, where the thermal equilibrium ensemble was prepared to the pseudo-pure state $|c_1^0\rangle|y_1^0\rangle|u_1^0\rangle$ by spatial averaging method.[17] Following the steps in the circuit, we could obtain the output $(|c_1^0\rangle|y_1^0\rangle|u_1^0\rangle + |c_1^1\rangle|y_1^0\rangle|u_1^1\rangle)/\sqrt{2}$. What we should do is to single out the result $|c_1^1\rangle|y_1^0\rangle|u_1^1\rangle$ in which the register $|u_1^1\rangle$ implies the solution to the single variable SAT problem $F = u_1$ and the second qubit $y_1$ has been nulled for later use.

We carry out the experiment on a Varian INOVA NMR spectrometer with the sample $^{13}$C-labelled alanine, i.e., $^{13}_{1}\mathrm{CH_3} - ^{13}_{2}\mathrm{CH(NH_2)} - ^{13}_{3}\mathrm{COOH}$. The three qubits are encoded in the carbons $^{13}_{1}$C, $^{13}_{2}$C and $^{13}_{3}$C, respectively, with $J$-coupling constants $J_{12} = 34.79$ Hz, $J_{23} = 54.01$ Hz and $J_{13} = 1.2$ Hz. The pulse sequences to prepare the pseudo-pure state are from Ref.[18]. The Hadamard gate can be realized by a single pulse $\pi/2$ along the $x$-axis and the CNOT gate is implemented by the pulse[17] $[\pi/2]_y^2 \rightarrow (1/4J) \rightarrow [\pi/2]_x^{1,2} \rightarrow (1/4J) \rightarrow [\pi]_x^{1,2} \rightarrow [\pi/2]_x^2$. Due to the weak measurement in NMR, we have no state collapse after measurement. Besides, only single quantum coherence can be detected in NMR. As a result, we have to employ some additional operations for detecting the output state $(|c_1^0\rangle|y_1^0\rangle|u_1^0\rangle + |c_1^1\rangle|y_1^0\rangle|u_1^1\rangle)/\sqrt{2}$. We may detect the second qubit directly by applying a $\pi/2$ readout pulse along the $x$-axis, yielding Fig.3(b). But for the first and third qubits, we need to disentangle them before measurement. To this end, we apply a CNOT gate, respectively, on the first (control) and second (target) qubits followed by another CNOT gate, respectively, on the second (control) and first (target) qubits to get the state $(|c_1^0\rangle|y_1^0\rangle|u_1^0\rangle + |c_1^0\rangle|y_1^1\rangle|u_1^1\rangle)/\sqrt{2}$. Then the first qubit can be read out, as shown in Fig.3(a). Similar steps applied to the third qubit result in the state $(|c_1^0\rangle|y_1^0\rangle|u_1^0\rangle + |c_1^1\rangle|y_1^1\rangle|u_1^0\rangle)/\sqrt{2}$ and the spectrum can be found in Fig.3(c).

The experimental results are in good agreement with our theoretical prediction and prove that the SAT problem could be solved by QC following the route of the DNAC. Some remarks must be addressed. First of all, the three-qubit NMR experiment we have carried out suffices to make a comprehensive test for our theory, because we have achieved the key aspects of our quantum implementation. Although the simplest case with three qubits to solve $F = (u_1)$ did not reflect the efficiency of QC implementation for SAT problem, we argue that, with more variables and clauses involved, the QC efficiency would be more and more evident, which could also be found in our later discussion about the computational complexity. Secondly, DNAC does not involve entanglement, whereas entanglement does appear in our quantum treatment, which, along with the state collapse in measurement, makes it possible for QC to have a speed-up in computation. The necessity of additional operations to disentangle the output qubits is not the intrinsic characteristic of our quantum mechanical treatment, but due to the unique feature of NMR technique. Anyway, those additional operations have not changed the essence of our implementation. Thirdly, although employed to solve SAT problems for some years, DNA computation has been lack of mathematical description. As a result, the DNA experiment implementing algorithms, although sometimes seems to be wonderful,[19] is usually discussed empirically. In this sense, our investigation of the relation between DNAC and QC actually presents a mathematical description of the DNAC operations, which is helpful for us to further understand the efficiency and the functions of DNAC.

We may simply assess the complexity of our quantum implementation of DNAC from Fig.2 and from more general case. The time complexity is $O(n)$ H gates, $O(6 \times m \times n)$ NOT gates, $O(2 \times m \times n)$ CNOT gates, and $O(m \times n + m)$ TOFF gates. The space complexity is $O(m + 3 \times n + 2)$ qubits, involving the ancillary qubits. However, readout is still an open question. Generally speaking, the readout requires exponential overhead, not only for bulk NMR systems, but also for other real qubit systems. For example, in our case, with more qubits involved, there will be more component states in a superposition. As a result, to single out our desired component state from the $n$-qubit system by projective measurement, the success rate is only $1/2^n$. A good way to obtain the desired component state with big probability from the superposition seems to be using the Grover search which singles out a desired state by amplifying the amplitude. We have noticed recent investigations on quantum search either theoretically or experimentally,[20−22] in which optimal implementation of the Grover search, full use of parallelism of QC and so on are intensively studied. We will also try to explore the search problem both theoretically and experimentally in the future.

In summary, we have experimentally demonstrated a quantum mechanical implementation of

DNAC to solve a simplest SAT problem by NMR techniques. Both QC and DNAC are hot topics as interdisciplinary subjects, and both of them have merits and drawbacks.[2,10,23] Our investigation, as a preliminary study, has presented relations between them, and we argue that it could enable us for not only a further exploration of quantum algorithms, but also a further understanding of DNAC from a brand-new angle.

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