Vol 18 No 12, December 2009
1674-1056/2009/18(12)/5173-06

Chinese Physics B

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

Ren Ting-Ting(任婷婷)[a)b)c)], Feng Mang(冯 芒)[a)†],
Chang Weng-Long(张云龙)[d)], and Luo Jun(罗 军)[a)b)]

[a)] *State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, the Chinese Academy of Sciences, Wuhan* 430071, *China*

[b)] *Center for Cold Atom Physics, the Chinese Academy of Sciences, Wuhan* 430071, *China*

[c)] *Graduate School of the Chinese Academy of Sciences, Beijing* 100049, *China*

[d)] *Department of Computer Science and Information Engineering, National Kaohsiung University of Applied Sciences, Kaohsiung* 80778, *China*

(Received 7 October 2008; revised manuscript received 29 June 2009)

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

*Project supported by the National Natural Science Foundation of China (Grant Nos 10774163 and 10574143), and the National Basic Research Program of China (Grant No 2006CB921203).

†Corresponding author. E-mail: mangfeng@wipm.ac.cn

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

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.

References

[1] Feynman R P 1961 *In Molecule* ed. Gilbert D H (New York: Reinhold Publishing Corporation) pp 282–285
[2] Lipton R 1995 *Science* **268** 542
[3] Dong R X and Yan X L 2007 *Chin. Phys.* **16** 2062
[4] Li M J, Liu X L, Ma S S and Xu H 2007 *Chin. Phys.* **16** 862
[5] Feynman R P 1982 *Int. J. Theor. Phys.* **21** 467
[6] Häffner H, Hänsel W, Roos C F, Benhelm J, Chek-al-kar D, Chwalla M, Körber T, Rapol U D, Riebe M, Schmidt P O, Becher C, Gühne O, Dür W and Blatt R 2005 *Nature* (London) **438** 643
[7] Lu C Y, Zhou X Q, Gühne O, Gao W B, Zhang J, Yuan Z S, Goebel A, Yang T and Pan J W 2007 *Nature Phys.* **3** 91
[8] Chuang I L, Vandersypen L M K, Zhou X L, Leung D W and Lloyd S 1998 *Nature* (London) **393** 143
Gulde S, Riebe M, Lancaster G P T , Becher C, Eschner J, Häffner H, Schmidt-Kaler F, Chuang I L and Blatt R 2003 *Nature* (London) **421** 48
[9] Nielsen M A and Chuang I L 2000 *Quantum Computation and Quantum Information* (Cambridge: Cambridge University Press)
[10] Adleman L 1994 *Science* **266** 1021
[11] Vadral V, Barenco A and Ekert A 1996 *Phys. Rev.* A **54** 147
[12] Vandersypen L M K and Chuang I L 2004 *Rev. Mod. Phys.* **76** 1037
[13] Wei D X, Luo J, Sun X P, Zeng X Z, Yang X D, Liu M L and Ding S W 2003 *Chin. Sci. Bull.* **48** 239
[14] Liu X M, Luo J and Sun X P 2007 *Chin. Phys. Lett.* **24** 3316
[15] Wei D X, Luo J, Yang X D, Sun X P, Zeng X Z, Liu M L, Ding S W and Zhan M S 2004 *Chin. Phys.* **13** 817
[16] Chuang I L, Gershenfeld N, Kubinec M G and Leung D W 1998 *Proc. R. Soc. London* A **454** 447
[17] Cory D G, Fahmy A F and Havel T F 1997 *Proc. Nat. Acad. Sci.* **94** 1634
Jones J Q 2001 *Prog. Nucl. Magn. Reson. Spectrosc.* **38** 325
[18] Cory D G, Price M D and Havel T F 1998 *Physica* D **120** 82
[19] Zhao J A, Qian L L, Liu Q, Zhang Z Z and He L 2007 *Chin. Sci. Bull.* **52** 1462
[20] Xiao L and Long G L 2002 *Phys. Rev.* A **66** 052320
[21] Guo H, Long G L and Li F 2002 *Commun. Theor. Phys.* **37** 424
[22] Liu W Z, Zhang J F and Long G L 2008 *Commun. Theor. Phys.* **49** 629
[23] Bennett C H, Bernstein E, Brassard G and Vazirani U 1997 *SIAM J. Comp.* **26** 1510