QUANTUM COMPUTING WITH BOSE OPERATORS

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Abstract. *One of the challenges for quantum computers, including the most promising for practical implementations NMR-based quantum computers, at the moment is to increase the number of qubits available for computation. Using the invariance of the spin projections operators under orthogonal reduction and orthogonal addition of the basis spin functions, the quantum computation at any number of qubits is proposed. It is showm that a quantum computer with N qubits can be characterized by the spin* $S = 2^{N-1} - 1/2$ *. The Hadamard gate in the two-Bose operators representation for a great number of qubits* ($N \to \infty$ *) has been determined.*

Key words: *quantum computer, qubit, NMR, Bose operators, Hadamard gate, expectation value.*

I. Introduction

The number of publications in the field of quantum informatics is in a continuous increasing that is caused by much larger possibilities of quantum computers comparatively with classical ones. The main difference between quantum and classical computers is due to the fact that the complete characterization of a register containing of N qubits (such as N coupled 1/2-spins) requires 2^N complex numbers, whereas a register of N classical bits is completely characterized by N integer (0 or 1). The logic gates of a quantum computer can perform logic operations on a qubits in different states at the same time, whereas a conventional bits in classical computer are limited to operations performed one after the other.

At present experimental approaches for the realization of quantum computers are connected with ion traps [1], quantum dots [2], Josephson contacts [3], endohedral fullerenes [4], liquid state NMR and solid state NMR/EPR [5, 6]. Even at the low level of three qubits the resulting experiments were sufficiently complicated to motivate the development and use of a host simplification technique and experimental methods to construct the quantum computer.

NMR spectroscopy has become well established as a tool for experimental investigation of quantum computation. Fundamental quantum gates, quantum algorithms, quantum error correction and other issues in quantum information theory have been demonstrated at the level of a few qubits using liquid state NMR systems at room temperature [7-20]. Among other methods the NMR spectroscopy is most advanced in the practical implementation of quantum algorithms. There are several publications (see for example [21-23]), which the construction of a NMR realization from the theoretical algorithm to the final spectrometer output and the algorithm result is described. As candidate for quantum computing, NMR is attractive because of the long coherence time exhibited by the spins and also due to complexity of logical operations that can be executed on modern NMR spectrometers. A molecule with N spin 1/2 nuclei can be visualized as an N-bit quantum computer, provided the spins are able to interact, one can manipulate their state in a desired fashion and there is a well-defined method of reading out the result of the computation [23]. NMR spectroscopy provides convenient methods for the controlled manipulations of nuclear spins, which are particularly well suited to act as qubits because of their isolation from the environment. However, a liquid NMR sample contains an ensemble of many identical spin systems and it is not possible to manipulate or to detect individual spin systems. Therefore, at the beginning of a computation, NMR quantum computers are commonly prepared in a "pseudo-pure" state, and ensemble-averaged expectation values are detected rather than the observables of individual spin systems [15,16]. The behavior of pseudo-pure states is similar in many respects to a pure ones. In particular, the pseudo-pure states can be described by a type of spinors, which evolve via unitary transformations under the Hamiltonian of NMR and whose expectation values are easily obtained from the corresponding ensemble-average expectation values. These spinors were called pseudo-spinors, to emphasize the fact that their physical interpretation differs from that of the spinors that describe isolated spin systems.

In this paper, the quantum computing based on two-Bose operators representation of the angular momentum for the case of a big number of qubits is presented.

II. Results

The Hilbert space of a single spin-$1/2$ particle (qubit) is spanned by the two mutually orthogonal basis states [5]

$$\begin{pmatrix}1\\0\end{pmatrix}=\left|\uparrow\right\rangle=\left|0\right\rangle \text{ and } \begin{pmatrix}0\\1\end{pmatrix}=\left|\downarrow\right\rangle=\left|1\right\rangle.$$

To obtain the basic states for a system of two qubits it is necessary to calculate the following Kronecker products of ket-vectors: $\left|00\right\rangle=\left|0\right\rangle\otimes\left|0\right\rangle$, $\left|01\right\rangle=\left|0\right\rangle\otimes\left|1\right\rangle$, $\left|10\right\rangle=\left|1\right\rangle\otimes\left|0\right\rangle$ and $\left|11\right\rangle=\left|1\right\rangle\otimes\left|1\right\rangle$. It is easy to show that these four Kronecker products can be mapped to the standard spinor basis of the spin $S=3/2$. Indeed, the Kronecker product $\otimes$ of an $m\times n$ matrix A with an $m'\times n'$ matrix **B** by definition is and $mm'\times nn'$ matrix given by

$$A\otimes B=\begin{pmatrix}a_{11}B & \dots & a_{1n}B\\ \dots & \dots & \dots\\ a_{m1}B & \dots & a_{mn}B\end{pmatrix},$$

where

$$A=\begin{pmatrix}a_{11} & \dots & a_{1n}\\ \dots & \dots & \dots\\ a_{m1} & \dots & a_{mn}\end{pmatrix}.$$

According to this definition, the basis vectors for a system of two qubits are given by

$$\left|00\right\rangle=\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\ \left|01\right\rangle=\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}0\\1\\0\\0\end{pmatrix},$$

$$\left|10\right\rangle=\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}0\\0\\1\\0\end{pmatrix},\ \left|11\right\rangle=\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

For a system of three qubits there are eight basis state $\left|0\right\rangle\otimes\left|00\right\rangle$, $\left|0\right\rangle\otimes\left|01\right\rangle$, $\left|0\right\rangle\otimes\left|10\right\rangle$, $\left|0\right\rangle\otimes\left|11\right\rangle$, $\left|1\right\rangle\otimes\left|00\right\rangle$, $\left|1\right\rangle\otimes\left|01\right\rangle$, $\left|1\right\rangle\otimes\left|10\right\rangle$ and $\left|1\right\rangle\otimes\left|11\right\rangle$ wich correspond to the basis states of a spin $S=7/2$. In the case of N qubits the basis vectors correspond to the eigent states of the spin projection operator S_Z, with the spin $S=2^{N-1}-\frac{1}{2}$.

It can be noticed that making a set of Kroneker products of spinors $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$ belonging to diffrent qubits, the spinor basis for the spin $S = 2^{N-1} - \frac{1}{2}$ can be obtained. However, it is not necessary to calculate the Kronecker products for each number N of qubits. It is sufficient to use the known standard basis vectors for the spin S at given number N of qubits. The values of S at different N are presented in the Table 1. Thus, in the case of N qubits there are 2^N spinor basis vectors corresponding to the spin $S = 2^{N-1} - \frac{1}{2}$. With increasing number of qubits the dimension of S_X, S_Y and S_Z matrices quickly increases (for exemple, at N = 10 the dimension of spin matrices is 1024×1024, $S = 1023/2$).

Table 1. Values of the effective spin S for different numbers N of qubits.

N	1	2	3	4	5	6	7	8	9	10	…	N
S	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{7}{2}$	$\frac{15}{2}$	$\frac{31}{2}$	$\frac{63}{2}$	$\frac{127}{2}$	$\frac{255}{2}$	$\frac{511}{2}$	$\frac{1023}{2}$	…	$2^{N-1} - \frac{1}{2}$

It is possible to show that all multi-qubit operations can be decomposed into one- and two-qubit operations [5]. On the other hand, there are the possibilities for quantum computing without such decomposition. This approach is based on the theorem about full reduction of the operator loads for the operators of angular momentum projections in the two-Bose operators representation [25]. As a consequence of this theorem, in the two-Bose operators representation the spin operators are invariant relative to orthogonal addition or orthogonal reduction of the spin space basis. Therefore, in this representation the operators $S_\pm = S_X \pm iS_Y$ and S_Z have the form

$$S_+ = a_1^+ a_2\,,\ S_- = (S_+)^+ = a_2^+ a_1\,,\ S_Z = \frac{1}{2}\left(a_1^+ a_1 - a_2^+ a_2\right) \tag{1}$$

independent of the spin value S. Here a_1^+ and a_2^+, a_2 are the operators of creation and annihilation of two different types of Bose-particles. These operators satisfy the commutation relations

$$\left[a_1, a_1^+\right] = \left[a_2, a_2^+\right] = 1\,,\ \left[a_1, a_2\right] = \left[a_1^+, a_2^+\right] = 0$$

and, what is more, satisfy the condition for the operator of total number of bosons

$$n = n_1 + n_2 = a_1^+ a_1 + a_2^+ a_2 = 2S\,, \tag{2}$$

which limits the number of Bose-particle states by means of which the spin wave functions of a system with the spin S are determined.

Since in the two-Bose operators representation the forms of S_+, S_- and S_Z operators does not depend on the spin S of the multi-qubit, specific features on N-qubits system are determined by the corresponding spin wave functions. For a system with the spin $S = 2^{N-1} - \frac{1}{2}$ these spin wave functions in the two-Bose operators representation are

$$\left|2^N - 1\right\rangle_1 |0\rangle_2,\ \left|2^N - 2\right\rangle_1 |1\rangle_2,\ \left|2^N - 3\right\rangle_1 |2\rangle_2, ...,\ |2\rangle_1 \left|2^N - 3\right\rangle_2,\ |1\rangle_1 \left|2^N - 2\right\rangle_2,\ |0\rangle_1 \left|2^N - 1\right\rangle_2, \tag{3}$$

where $\left|2^N - k\right\rangle_i$ is the wave function of $\left(2^N - k\right)$-th excited boson state containing $2^N - k$ bosons of the i-th type ($i = 1,2$) and $|0\rangle$ is the vacuum state of the i-th Bose field ($i = 1,2$). On the basis of a set of pair products of different boson wave functions $|k\rangle_1$ and $|l\rangle_2 \left(k + l = 2^N - 1\right)$ from (3) the basis functions for the systems of one, two, etc. qubits can be easily obtained. The basis functions from (3) were obtained as a particular case of general formula for spin wave functions in the two-Bose operators representation [24, 26]:

$$\left|S,M\right\rangle = \frac{1}{\sqrt{(S+M)!(S-M)!}}\left(a_1^+\right)^{S+M}\left(a_2^+\right)^{S-M}\left|0\right\rangle, \tag{4}$$

taking into account the kinematic condition (2) for the spin $S = 2^{N-1} - \frac{1}{2}$. In (4) M is the eigenvalue of the operator S_Z.

Now it is clear that for quantum computing by means of the creation operators $\left(a_1^+, a_2^+\right)$ and annihilation operators $\left(a_1, a_2\right)$ of two Bose fields it is necessary:

- to transfer the spin operators S_X, S_Y and S_Z into two-Bose operators representation;
- to use the spin wave functions (3) in the two-Bose operators representation.

As an example, let us consider the Hadamard gate. In the case of one qubit the Hadamard gate H [5] is defined by

$$H_1 = \frac{1}{\sqrt{2}}(X + Z), \tag{5}$$

where

$$X = 2S_X,\ Z = 2S_Z. \tag{6}$$

Taking into account (1) and (6), the Hadamard gate from (5) in the two-Bose operators representation is

$$H_1 = \frac{1}{\sqrt{2}}\left[a_1^+(a_1 + a_2) + a_2^+(a_1 - a_2)\right]. \tag{7}$$

The matrix of the operator H_1 from (7), which was found by means of basis functions $\left|1\right\rangle_1\left|0\right\rangle_2$ and $\left|0\right\rangle_1\left|1\right\rangle_2$, is given by

$$H_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix},$$

which coincides with the result obtained using the spinor formalism.

For two qubits the Hadamard gate is

$$H_2 = H_1 \otimes H_1 = \frac{1}{2}(X + Z)\otimes(X + Z) \tag{8}$$

In the two-Bose operators representation the operator H_2, taking into account (7) and (8), have the form

$$H_2 = \frac{1}{2}\left[a_1^+(a_1 + a_2) + a_2^+(a_1 - a_2)\right]\otimes\left[a_1^+(a_1 + a_2) + a_2^+(a_1 - a_2)\right] \tag{9}$$

The matrix H_2 defined in the spinor basis $\left\{\left|3/2\right\rangle, \left|1/2\right\rangle, \left|-1/2\right\rangle, \left|-3/2\right\rangle\right\}$, that is equivalent to two-Bose operators basis $\left\{\left|3\right\rangle_1\left|0\right\rangle_2, \left|2\right\rangle_1\left|1\right\rangle_2, \left|1\right\rangle_1\left|2\right\rangle_2, \left|0\right\rangle_1\left|3\right\rangle_2\right\}$, is

$$H_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1 & 1 & 1\\ 1 & -1 & 1 & -1\\ 1 & 1 & -1 & -1\\ 1 & -1 & -1 & 1\end{pmatrix}.$$

In the case of three qubits we have

$$H_3 = H_2 \otimes H_1 = H_1 \otimes H_1 \otimes H_1.$$

In the spinor basis, the H_3 matrix is

$$H_3 = \frac{1}{2\sqrt{2}}(X+Z)\otimes(X+Z)\otimes(X+Z)$$

while in the two-Bose operators representation it is

$$H_3 = \frac{1}{2\sqrt{2}}\left[a_1^+(a_1+a_2)+a_2^+(a_1-a_2)\right]\otimes\left[a_1^+(a_1+a_2)+a_2^+(a_1-a_2)\right]\otimes\left[a_1^+(a_1+a_2)+a_2^+(a_1-a_2)\right] \quad (10)$$

The matrix H_3 defined in the spinor basis $\{|7/2\rangle, |5/2\rangle, |3/2\rangle, |1/2\rangle, |-1/2\rangle, |-3/2\rangle, |-5/2\rangle, |-7/2\rangle\}$ or in the equivalent two-Bose operators basis $\{|7\rangle_1|0\rangle_2, |6\rangle_1|1\rangle_2, |5\rangle_1|2\rangle_2, |4\rangle_1|3\rangle_2, |3\rangle_1|4\rangle_2, |2\rangle_1|5\rangle_2, |1\rangle_1|6\rangle_2, |0\rangle_1|7\rangle_2\}$, is

$$H_3 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{pmatrix}.$$

For any number N of qubits the Hadamard operator H_N is

$$H_N = H_1 \otimes H_1 \otimes H_1 \otimes \ldots \otimes H_1,$$

where the operator H_1 is found in this Kronecker product N times. On the other hand, the operator H_N is given by recursive formula

$$H_N = \frac{1}{\sqrt{2}}\begin{pmatrix} H_{N-1} & H_{N-1} \\ H_{N-1} & -H_{N-1} \end{pmatrix}. \quad (11)$$

In the spinor basis the operator H_N is

$$H_N = \frac{1}{2^{N/2}}(X+Z)\otimes(X+Z)\otimes(X+Z)\otimes\ldots\otimes(X+Z),$$

while in the two-Bose operators representation it is

$$H_N = \frac{1}{2^{N/2}}\left[a_1^+(a_1+a_2)+a_2^+(a_1-a_2)\right]\otimes\ldots\otimes\left[a_1^+(a_1+a_2)+a_2^+(a_1-a_2)\right]. \quad (12)$$

All calculations using the operators from (7), (9), (10) and (12) must be performed taking into account the kinematic condition (2).

The matrix H_N is defined in the spinor basis $\left\{\left|2^{N-1}-\frac{1}{2}\right\rangle, \left|2^{N-1}-\frac{3}{2}\right\rangle, \ldots, \left|-2^{N-1}+\frac{3}{2}\right\rangle, \left|-2^{N-1}+\frac{1}{2}\right\rangle\right\}$ or in the equivalent two-Bose operators basis from (3). Using the formula (11) it is easy to show that H_N^2 is the identity operator ($H_N^2 = 1$).

By this way, we can find the transformation properties of the spin basis functions in the two-Bose operators representation for the spin $S = 2^{N-1} - \frac{1}{2}$ under action of Hadamard operator in the case of any number N of qubits. In particular, if $N = 77$ then the total number of bosons of first and second types, which is necessary for realization of the two-Bose operators representation in the case of spin $S = 2^{76} - \frac{1}{2} \sim 2^{76}$, is $N \sim 10^{23}$. At such large number of qubits the kinematic condition (2) does not play such an important role as at low values of the spin *S* and, respectively, for small number of qubits. In this case the number of spin states is so large that it can be considered infinite, as is the number of degrees of freedom of the boson field.

The transition from spinor representation to two-Bose operators one must be done for spin wave functions, spin operators, Zeeman operator, evolution operator, spin dependent density operator, etc.

The quantum information processing using two-Bose operators representation of angular momentum is an effective processing in the case of high number *N* of qubits because in this case it is possible to use the Wick's theorem [27] that simplifies calculations.

III. Conclusions

The NMR-based quantum computer is promising technique to illustrate and explore ideas in quantum computation. It is caused by demonstrating experimentally various selective pulse and implementations of pseudo-pure states, novel quantum logic gates and quantum algorithms. The easy with which quantum circuits can be implemented in NMR experiments and the facility with which spin dynamics can be manipulated using a variety of techniques is a major advantage of NMR-based quantum computers.

However, one of the challenges for NMR spectroscopists at the moment is to increase the number of qubits available for computation. A set of important problems in quantum computing such as implementing quantum algorithms with a greater number of qubits, constructing error correcting circuits for fault-tolerant computing and performing large scale quantum simulations awaiting their solution in the near future. In the case of a large number of qubits the quantum computing based on two-Bose operators representation of the angular momentum can be preferable because in this case the well developed methods of quantum electrodynamics can be used.

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