A polynomial-time solution to the parity problem on an NMR quantum computer

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Abstract

An efficient quantum algorithm is proposed to solve in polynomial time the parity problem, one of the hardest problems both in conventional quantum computation and in classical computation, on NMR quantum computers. It is based on the quantum parallelism principle in a quantum ensemble, the selective decoherence manipulation, and the NMR phase-sensitive measurement. The quantum circuit for the quantum algorithm is designed explicitly.

1. Introduction

It is well known that the parity problem is one of the hardest problems [1, 2]. These hard problems [1-4] including the parity problem, majority problem, and some iteration problem, etc., can not be solved efficiently both on the classical and quantum computers in polynomial time so far. It has been shown that quantum computers can achieve no more than a polynomial speedup over the classical computers in solving these hard problems, implying that a quantum computer cannot outperform a classical computer in solving these problems [1, 2]. On the other hand, since nuclear magnetic resonance (NMR) technique [5, 6] has been proposed to implement in experiment quantum computation [7, 8], there are some difficulties, limits, and questions in NMR quantum computation [9, 10], although a great and rapid progress has been achieved and a great flow of the work has been reported in past several years. Due to too low spin polarization in a spin ensemble at room temperature [9] it can not be certain up to now from quantum mechanical principle whether NMR quantum computation is a real quantum computation and can be more powerful than the classical computation. Some peoples [11-13] even claimed from the view point of the quantum entanglement theory that NMR quantum computers are not in fact real quantum computers, and suspect whether or not NMR quantum computation based
on the effective pure states [7, 8] is as powerful as the quantum computation based on the pure quantum states also owing to the two main drawbacks, that is, an exponent reduction of NMR signal intensity as the qubit number and a high cost for the preparation of the initial effective pure state on NMR quantum computation. However, most recently an efficient quantum algorithm running on the NMR quantum computers is proposed to solve in polynomial time the unsorted quantum search problem [14]. It is well known that the conventional quantum search algorithm, i.e., the Grover algorithm, based on the pure quantum states [15] or the effective pure states [16] cannot solve the search problem in polynomial time, although it is a quadrup speedup algorithm over the classical search algorithms. Therefore, the new quantum search algorithm shows that quantum algorithms on the NMR quantum computers are not only as powerful as on the conventional quantum computers based on the pure quantum states but also some quantum computations running on the NMR quantum computer can be more powerful than running on the conventional one. This algorithm is based on the quantum parallelism principle in quantum ensembles, the selective decoherence manipulation, and NMR phase sensitive measurement [14]. In this paper I further show that there is an efficient quantum algorithm to solve the parity problem in polynomial time on the NMR quantum computers. It is still based on the quantum parallelism principle in quantum ensembles, the selective decoherence manipulation, and NMR phase sensitive measurement. The present quantum algorithm to efficiently solve the parity problem in polynomial time supports powerfully the belief that the NP hard problems can be efficiently solved in polynomial time on quantum computers and quantum computers can outperform eventually the classical computers.

2. Quantum parallelism in a quantum ensemble

The quantum parallelism is one of the most basic principles in quantum computation [17]. In principle, the quantum parallelism offers the possibility that quantum computation can be more powerful than the classical computation, although it is usually difficult to extract the desired computational output from a quantum system in quantum computation directly by the quantum mechanical measurement [18]. The quantum parallelism may be understood simply through the process that superposition of a quantum system is acted on by a unitary transformation of quantum computation. Since a quantum system can be at any superposition which can be a linear sum of the usual quantum computational bases, while number and functional
operation in mathematics usually may be represented by the computational bases and the unitary transformation, respectively, in quantum computation, then performing quantum mechanically the unitary transformation of the functional operation on the superposition means really that the functional operation is performed in a parallel form with all input numbers represented by those computational bases of the superposition. Because quantum computation is a reversible computational process [19] an arbitrary quantum state of the quantum system is equivalent unitarily to a computational basis or any other quantum state of the system, that is, any pair of quantum states of the system can be unitarily converted completely each other in quantum computation [20] when there are not quantum measurement and decoherence process during the quantum computation. Now, if the superposition is expressed as a unitary transformation acting on some usual computational basis, the above functional operation process really can start at the computational basis instead of the superposition. However, this does not mean that there is not the quantum parallelism in the computational process even when the initial input state is not superposition. This is because superposition of the quantum system is usually created during the unitary transformation of the functional operation. Therefore, in fact the quantum parallelism is also characterized by unitary transformation besides superposition. Due to this fact sometime the initial input state is included in a quantum algorithm [21]. However, it is key important to separate the initial input state representing in mathematics number and the unitary transformation representing the functional operation mathematically when the quantum parallelism principle is extended to a quantum ensemble and can be able to play an important role in quantum computation. In general, a molecule spin system and its spin ensemble composed of the molecule spin system obey the unitary dynamics governed by the same spin Hamiltonian in nuclear magnetic resonance spectroscopy [5, 6]. This point is very helpful for quantum computation making a transition from the quantum spin system version to the spin ensemble version. It has been shown that any unitary transformation of quantum computation can be constructed with the spin Hamiltonian of a spin system [22]. Then the unitary transformation is still available and takes the same form when quantum computation is carried out in the spin ensemble with the same spin Hamiltonian of the molecule spin system. The significant difference between the spin system and its ensemble is that there are mixed states in addition to the pure quantum states in the spin ensemble. However, just due to the fact that a spin ensemble can be in a mixed state, the spin ensemble can provide
the quantum parallelism principle with a much larger space for it to bring into play in quantum computation when the unitary transformation and the initial input state are independent on each other in quantum computation. This is because the initial input state of the quantum computation may be any mixed state in addition to the pure quantum state in a spin ensemble.

In a quantum system with $n$ qubits there are $N = 2^n$ usual computational bases or $N$ any other eigenbases in the $N$-dimensional Hilbert space of the quantum system, and any superposition of the quantum system can be expressed as a linear sum of the $N$ eigenvectors in the vector representation. In the matrix representation any superposition of the quantum system is still expressed as a linear sum of $N$ linearly independent quantum states which are now represented by matrices, but this matrix representation just gives the same information of the quantum system as the vector representation provides. For example, the effective pure state in a spin ensemble [7, 8] provides a faithful matrix representation for the pure quantum state of the spin system in the spin ensemble, but it does not give more information than the pure quantum state in quantum computation. However, any superposition of a spin ensemble, that is, any mixed state or any density operator of a spin ensemble must be expanded as a sum of any $4^n$ linearly independent matrix bases in the $4^n$-dimensional Liouville space of the spin ensemble [5]. A mixed state is not always able to be unitarily transferred completely into another mixed state in a spin ensemble, and this is quite different from the case in a quantum system in quantum computation. If any unitary transformation and the initial input state are independent on each other in a quantum algorithm whose quantum circuit is constructed with the spin Hamiltonian of a spin system or its spin ensemble, any mixed state of the spin ensemble can be used as the initial input state of the quantum algorithm run on the spin ensemble. Then, the initial input state of the quantum algorithm can be selected from the larger $4^n$-dimensional Liouville space of the spin ensemble instead of the smaller $2^n$-dimensional Hilbert space of the spin system. This could be helpful to design efficient quantum algorithms to solve some hard problems on a spin ensemble.

How to solve mathematical problems in a spin ensemble like in a quantum system? The well-known scheme is based on the effective pure state [7, 8], but according to the scheme the mixed states in a spin ensemble really do not play an important role in the quantum computation. A possible scheme proposed here is that the complete information of the problems to be solved first is contained or hidden in unitary transformation of quantum compu-
tation or its corresponding effective Hamiltonian and/or the mixed states in the spin ensemble, and the simpler and better one is that only the unitary transformation contains the complete information of the problem to be solved. By choosing the suitable initial mixed states one runs the quantum algorithm on the spin ensemble, and then extracts the desired information of the problem by NMR phase-sensitive measurement technique [5, 6]. The latter scheme has been used to find the efficient quantum search algorithm on NMR quantum computers [14].

3. Selective decoherence manipulation

All the coherent and the noncoherent components (the longitudinal magnetization and spin order components in nonequilibrium state) in a spin ensemble decay irreversibly as time and at the same time the spin ensemble returns to the thermal equilibrium state irreversibly, but their decay rates are quite different [5, 6]. For example, in a spin ensemble the longitudinal relaxation time is always longer than the transverse relaxation time, and for some macromolecules the longitudinal relaxation time can be even hundred and thousand times longer than the transverse relaxation time. The important fact is that the decay rates for some coherent and noncoherent components in a spin ensemble can be manipulated and controlled externally. For example, the nonzero-order multiple-quantum coherences including the transverse magnetizations are much sensitive to the inhomogeneous external magnetic field but the longitudinal magnetizations are not [5, 6]. Then one can make use of the inhomogeneous external magnetic field, for example, a gradient magnetic field [6], to control the decay of these multiple-quantum coherences, so that at a short time these coherent components are cancelled but only the zero-quantum coherences and the longitudinal magnetizations and spin order components almost keep unchanged. Finally, the residual zero-quantum coherences can be cancelled by the zero-quantum dephasing pulse [24] or z-filter [5, 6, 25] so that only the longitudinal magnetization and spin order components are retained selectively in the spin ensemble. Such selective decoherence manipulation has been used extensively in nuclear magnetic resonance experiments. In quantum computation the quantum measurement is also a selective decoherence manipulation. The quantum state measured is retained but any other states decay to zero quickly in a quantum system when performing quantum measurement. The importance is how to exploit in a positive manner the selective decoherence manipulation to help to find new polynomial-time quantum algorithms in quantum computation. In quantum
computation the final goal is to extract the desired information of the problem to be solved by a quantum algorithm from the quantum system, but one need not obtain the complete information of the quantum system. Therefore, one may use properly the selective decoherence manipulation to cancel the undesired information but obtain valuable information which is sufficient to solve the problem. The spin ensemble provides a very suitable place to perform the selective decoherence manipulation for quantum computation since nuclear magnetic resonance technique is well-developed at present. The massive quantum parallelism makes it possible for quantum computation outperforming classical one, but the desired computational output could not be obtained easily due to the limit of the quantum measurement principle in a quantum system. However, since the selective decoherence manipulation in a spin ensemble can be performed more conveniently, the undesired coherent and noncoherent components created in quantum computation in a spin ensemble could be cancelled and as a consequence, the desired computational results could be detected conveniently by the NMR phase-sensitive measurement technique [14]. Here, the selective decoherence manipulation is a positive effect in quantum computation. Though the decoherence effect is usually a negative effect on quantum computation and need to be overcome, the selective decoherence manipulation could be useful to help finding new efficient quantum algorithms. For example, most recently an efficient quantum search algorithm [14] based on the selective decoherence manipulation is proposed on the NMR quantum computers.

4. The quantum algorithm to solve efficiently the parity problem

The parity problem can be outlined briefly below. Given a function \( f(x) \) which is defined on the integers \( x: 0 \leq x \leq N - 1 \ (N = 2^n) \). For any \( x \) \((0 \leq x \leq N-1)\) the function \( f(x) \) can only take either +1 or -1. The parity of the function \( f(x) \) can be defined as [1]

\[
par(f) = \prod_{x=0}^{N-1} f(x)
\]

(1)

where \( f(x) = \pm 1, \ x = 0, 1, ..., N-1 \). The parity problem of the function \( f(x) \) is how to determine the parity function \( par(f) \). Obviously, the parity function \( par(f) \) can only take either +1 or -1. To determine the parity problem in classical computation one needs to call \( N \) times the function \( f(x) \) so that \( f(x) \) can be known for each \( x \) value and hence the parity function \( par(f) \) can be
determined from Eq.(1). In quantum computation evaluation of the function $f(x)$ over all the $x$ values $0 \leq x \leq N - 1$ can be performed simultaneously by only one call of the functional operation of $f(x)$ on the superposition of the quantum system due to the quantum parallelism, but the final result, that is, all values of the function $f(x)$, can not be extracted simultaneously due to the limit of quantum mechanical measurement. As a result, the cost to solve the parity problem on a quantum computer is not really much lower than on a classical computer, implying that quantum computers can not outperform classical computers in determining the problem. However, the parity problem is a global-type or collective-type problem but not an individual one of the function $f(x)$. Perhaps people could not evaluate each value of the function $f(x)$ over all $x$ values but can determine the parity function (1).

First of all, the unitary transformation corresponding evaluation of the function $f(x)$ is introduced. This unitary operation is the oracle unitary operation in the quantum algorithm to solve the parity problem. Assume that the evaluation of the function $f(x)$ can be expressed by performing the oracle unitary operation $U_f$ on any quantum state $|x\rangle|S\rangle$ in a quantum system,

$$U_f|x\rangle|S\rangle = f(x)|x\rangle|S\rangle = \exp(-i\pi g(x))|x\rangle|S\rangle \quad (2)$$

where the auxiliary quantum state $|S\rangle$ must be chosen properly [1, 14, 18] so that equation (2) holds, and the function $g(x)$ is defined by $f(x) = \exp(-i\pi g(x))$, that is, $g(x) = 0$ if $f(x) = 1$; $g(x) = 1$ if $f(x) = -1$. When the oracle unitary operation $U_f$ acts once on any superposition of the quantum system all the values of the function $f(x)$ over all $x$: $0 \leq x \leq N - 1$ are evaluated simultaneously,

$$U_f \sum_{x=0}^{N-1} a_x|x\rangle|S\rangle = \sum_{x=0}^{N-1} a_x f(x)|x\rangle|S\rangle. \quad (3)$$

However, these function values are not simultaneously observable in the quantum system due to the limit of the quantum mechanical measurement. It has been shown that to determine certainly the parity problem on a quantum computer one needs to execute around $N/2$ times the oracle unitary operation $U_f$ [1, 2]. Equation (3) shows that the oracle unitary operation $U_f$ is independent upon any quantum state $|x\rangle$ of the work qubits $I$ (hereafter the symbol $I$ denotes the work qubits) in the quantum system but related to the auxiliary quantum state $|S\rangle$ (hereafter the symbol $S$ denotes the auxiliary qubits).

In order to construct the explicit equivalent form for the oracle unitary operation $U_f$ one may use the selective phase-shift operations $C_s(\theta)$ to express
the oracle unitary operation $U_f$. The selective phase-shift operation $C_x(\theta)$ is a diagonal unitary operator of the longitudinal magnetization and spin order operator subspace and defined as [14, 22]

$$C_x(\theta) = \exp(-i\theta D_s)$$

where the diagonal operator $D_s$ is defined as $D_s = \text{diag}(0, ..., 0, 1, 0, ..., 0)$, that is, $(D_s)_{ss} = 1$ for index $s$ and $(D_s)_{rr} = 0$ for any other index $r \neq s$. Note that when the selective phase-shift operation $C_x(\theta)$ acts on any quantum state $|r\rangle|S\rangle$ a phase shift $\exp(-i\theta)$ is created only when the index $r = x$, otherwise the quantum state $|r\rangle|S\rangle$ keeps unchanged, $C_x(\pi g(x))|r\rangle|S\rangle = \exp(-i\pi g(x)\delta_{rx})|r\rangle|S\rangle = \begin{cases} |r\rangle|S\rangle \quad \text{if } r \neq x, \\ f(x)|x\rangle|S\rangle \quad \text{if } r = x, \end{cases}$

and also note that any pair of the selective phase-shift operations commute each other. It can be seen from Eqs.(2) and (3) that the oracle unitary operation $U_f$ is really equivalent to the product of all $N$ selective phase-shift operations $C_x(\pi g(x)), x = 0, 1, ..., N - 1$,

$$U_f = \prod_{x=0}^{N-1} C_x(\pi g(x)).$$

In a more general case, in the present quantum algorithm the oracle unitary operation $U_f$ of Eq.(5) can be replaced with the more general oracle unitary operation $U_o(\theta)$ which is the product of the $N$ selective phase-shift operations $C_x(\theta g(x)), x = 0, 1, ..., N - 1, \text{ with any phase angle } \theta$ by choosing properly the auxiliary quantum state $|S\rangle = |0\rangle|1\rangle$ [14]

$$U_o(\theta) = U_f V(\theta) U_f = \prod_{x=0}^{N-1} C_x(\theta g(x)).$$

Note that the function $g(x) = 0, 1$ for $f(x) = 1, -1$, respectively, as shown in Eq.(2). The parity function $\text{par}(f)$ of Eq.(1) can be expressed as

$$\text{par}(f) = \prod_{x=0}^{N-1} f(x) = \prod_{x=0}^{N-1} \exp(-i\pi g(x)) = \exp(-i\pi \sum_{x=0}^{N-1} g(x)).$$

Define the integer phase parameter $G$ as

$$G = \sum_{x=0}^{N-1} g(x).$$

Obviously, $\text{par}(f) = +1$ if the integer phase parameter $G$ is an even number and $\text{par}(f) = -1$ if $G$ is an odd number. Therefore, the parity problem is really determined completely by the parity of the integer phase parameter $G$. Obviously, the integer phase parameter $G$ is a global or collective quantity. Its parity may be determined without knowing each individual value of the function $f(x)$ and hence the parity problem of the function $f(x)$ could be solved efficiently without knowing all the functional values $f(x)$ in advance.

In the above the oracle unitary operations $U_f$ of the functional operation

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$f(x)$ and $U_o(\theta)$ are introduced in a quantum system. Now to extend these oracle unitary operations to the ensemble composed of the quantum system the auxiliary quantum states $|S\rangle$ in the quantum system must be kept unchanged or be replaced by their corresponding equivalent effective pure states [23] in the quantum ensemble because the oracle unitary operations are related to the auxiliary quantum states $|S\rangle$, as can be seen in Eqs.(2), (3) and (6), but the quantum state $|x\rangle$ of the work qubits $I$ can be replaced by any mixed state or density operator of the ensemble [14].

To describe conveniently the evolution process of the quantum spin system or its spin ensemble under the action of the oracle unitary operation $U_o(\theta)$ (6) one needs to exploit the following general unitary transformation when the selective phase-shift operation $C_s(\theta)$ acts on any density operator $\rho_I(0)$ of the work qubits $I$ of the spin ensemble [26]:

$$C_s(\theta)\rho_I(0)C_s(\theta)^{-1} = \rho_I(0) - (1 - \cos \theta)[\rho_I(0), D_s]_+ + i \sin \theta[\rho_I(0), D_s] + [(1 - \cos \theta)^2 + \sin^2 \theta]D_s\rho_I(0)D_s$$  \hspace{1cm} (9)

where the commutation $[\rho_I(0), D_s]_+ = \rho_I(0)D_s + D_s\rho_I(0)$ and $[\rho_I(0), D_s] = \rho_I(0)D_s - D_s\rho_I(0)$. With the help of the unitary transformation (9) and the explicit expression (6) of the oracle unitary operation $U_o(\theta)$ one can obtain easily the following unitary transformation when the oracle unitary operation $U_o(\theta)$ acts on any density operator $\rho_I(0)|S\rangle\langle S|$ of the ensemble

$$U_o(\theta)\rho_I(0)U_o(\theta)^{-1} = \rho_I(0) - (1 - \cos \theta)[\rho_I(0), \sum_{s=0}^{N-1} g(s)D_s]_+ + i \sin \theta[\rho_I(0), \sum_{s=0}^{N-1} g(s)D_s] + [(1 - \cos \theta)^2 + \sin^2 \theta] \sum_{s=0}^{N-1} \sum_{t=0}^{N-1} g(s)g(t)D_s\rho_I(0)D_t.$$  \hspace{1cm} (10)

Here, without confusion the auxiliary pure quantum state or effective pure state $|S\rangle\langle S|$ is omitted. Equation (10) is the basic unitary transformation to analyze the quantum algorithm to solve efficiently the party problem on an NMR quantum computer. The initial density operator $\rho_I(0)$ must be related to each quantum state $|x\rangle$ ($x = 0, 1, ..., N - 1$), otherwise it keeps unchanged under the action of the selective phase-shift operation $C_s(\theta)$, $C_x(\theta)\rho_I(0)C_x(\theta)^{-1} = \rho_I(0)$, and as a result, one may not determine certainly the parity function of Eq.(1). One of the proper initial density operators in a spin ensemble may be

$$\rho_I(0) = \sum_{k=1}^{n} \varepsilon_k I_k$$  \hspace{1cm} (11)

where $\varepsilon_k$ is the spin polarization parameter of spin $k$ and the term proportional to the unity operator is omitted without losing generality. It has
proved that the density operator $\rho_I(0)$ of Eq.(11) are related to all the quantum states $|x\rangle$ of the spin system in the spin ensemble [14]. Furthermore, it is convenient to employ the unit-number vector representation \{a_k^s\} [14] to analyze the unitary transformation (10). In the unit-number vector representation the diagonal operator $D_s$ can be expressed as [14]
\[
D_s = (\frac{1}{2}E_1 + a_k^s I_{1z}) \otimes \ldots \otimes (\frac{1}{2}E_k + a_k^s I_{kz}) \otimes \ldots \otimes (\frac{1}{2}E_n + a_n^s I_{nz}).
\]
Assume that the work qubits $I$ are prepared initially at the density operator of Eq.(11) and the auxiliary qubit $S$ is in the quantum state $|S\rangle\langle S|$ [23] in the spin ensemble. Then make the oracle unitary operation of $U_o(\theta)$ on the spin ensemble. The spin ensemble will evolve according to the following unitary transformation obtained easily from Eq.(10):
\[
U_o(\theta) \sum_{k=1}^{n} \varepsilon_k I_{ky} U_o(\theta)^{-1} = \sum_{k=1}^{n} \varepsilon_k I_{ky} - (1 - \cos \theta) \sum_{k=1}^{n} g(s) \varepsilon_k I_{ky} \otimes \ldots \otimes (\frac{1}{2}E_k + a_k^s I_{kz}) \otimes \ldots \otimes (\frac{1}{2}E_n + a_n^s I_{nz}) - \sin \theta \sum_{k=1}^{n} g(s) \varepsilon_k I_{ky} \otimes \ldots \otimes (\frac{1}{2}E_k + a_k^s I_{kz}) \otimes \ldots \otimes (\frac{1}{2}E_n + a_n^s I_{nz})
\]
\[
+ [(1 - \cos \theta)^2 + \sin^2 \theta] \sum_{k=1}^{n} g(s) g(t) \varepsilon_k I_{ky} \otimes \ldots \otimes (\frac{1}{2}(1 + a_k^{s_1} a_k^{s_2}) E_1) \otimes \ldots \otimes (\frac{1}{2}(1 + a_k^{s_1} a_k^{s_2}) E_n) \}
\]
\[
(13)
\]
The mixed state of Eq.(13) of the spin ensemble after the action of the oracle unitary operation of $U_o(\theta)$ is quite complicated, but it can be simplified by the selective decoherence manipulation. First, a hard 90 degree pulse along y-axis direction is applied to all the spins of the work qubits $I$ of the spin ensemble and then a purge pulse [5, 6, 24, 25], that consists of the z-gradient field used to cancel all the nonzero multiple-quantum coherences including single-quantum coherences, and the zero-quantum dephasing pulse [24] used to cancel all the zero-quantum coherences, is applied to cancel all the undesired multiple-quantum coherences but only the longitudinal magnetization and spin order components keep unchanged. Then the final density operator is reduced to the form
\[
\rho_f = (2/N) \sum_{k=1}^{n} \varepsilon_k I_{kz} \langle \sum_{s=0}^{N-1} g(s)a_k^s \rangle = (2/N) \sum_{k=1}^{n} \varepsilon_k P_k I_{kz}
\]
(14)
where the phase angle \( \theta \) in the oracle unitary operation \( U_o(\theta) \) is taken as 90 degree. The density operator \( \rho_f \) of Eq.(14) determines the final observable NMR signal of any spin \( k \) \((k = 1, 2, ..., n)\) of the spin system in the spin ensemble, and the intensity of the NMR signal of the spin \( k \) is proportional to the sum \( P_k \), which is an integer defined by
\[
P_k = (\sum_{s=0}^{N-1} g(s) a_k^s) = \sum_t a_t^k
\]  
(15)
where the latter equality holds due to the fact that the function \( g(s) = 0, 1 \) for any index \( s \), and the second sum (the index \( t \)) runs over only those indexes \( s \) with \( g(s) = 1 \). It turns out easily that the integer \( P_k \) can take any integer from \(-N/2\) to \(N/2\) since \( a_k^t = \pm 1 \) for any indexes \( k \) and \( t \), and a half of all \( N \) unity numbers \( \{a_k^t\} \) take +1 for any given index \( k \). It follows from Eq.(15) that the parity of the integers \( P_k \) \((k = 1, 2, ..., n)\) is determined uniquely by that of the integer phase parameter \( G \) and in turn, the parity of the integer phase parameter \( G \) is also determined uniquely by that of the integer \( P_k \), that is, if the integer phase parameter \( G \) is an even number each integer \( P_k \) must also be an even number, and if \( G \) is an odd number each \( P_k \) is an odd number too. Now, if every integer \( P_k \) is an odd number it follows from the density operator \( \rho_f \) of Eq.(14) that the NMR signal for any spin \( k \) \((k = 1, 2, ..., n)\) of the spin system in the ensemble always has a nonzero intensity. Obviously, if there is zero-intensity NMR signal of the density operator \( \rho_f \) of Eq.(14) for any arbitrary spin \( k \) of the spin system in the ensemble it can be certain that all the integers \( \{P_k\} \) are even numbers (including zero) and hence the integer phase parameter \( G \) is also an even number. However, there is another possibility that the NMR signal of the density operator \( \rho_f \) of Eq.(14) for all the spins in the ensemble can have nonzero intensity even when all the integers \( \{P_k\} \) are nonzero even numbers. It is clear that the parity problem can be solved efficiently by the above process only when the NMR signal of the density operator (14) for one spin of the spin system at least in the ensemble has a zero intensity. If the NMR signal of the density operator \( \rho_f \) of Eq.(14) for all spins in the ensemble have nonzero intensities the above process can not determine certainly the parity problem. To solve this problem one needs to modify the above quantum algorithm. First, a phase-shift operation \( U_M(-\pi/2) \) is introduced. This known phase-shift unitary operation is not an oracle unitary operation and is applied only on the work qubits \( I \) of the ensemble. It is defined by
\[
U_M(-\pi/2) = \prod_I C_I(-\pi/2).
\]  
(16)
This phase-shift unitary operation is the product of $M$ selective phase-shift operations $C_l(-\pi/2)$, while these selective phase-shift operations are given in advance and are required to meet some constraint that will be stated below. It turns out easily that the phase-shift unitary operator $U_M(-\pi/2)$ commutes with the oracle unitary operator $U_o(\theta)$: $[U_M(-\pi/2),U_o(\theta)] = 0$.

Now a modified quantum algorithm to solve the parity problem is given below. One first makes an oracle unitary operation of $U_o(\pi/2)$ on the initial density operator $\rho_I(0)$ of Eq.(11) and then applies the known phase-shift unitary operation $U_M(-\pi/2)$ to the ensemble, then adds y-axis direction 90 degree pulse 90° and a purge pulse just as the above process. It is easy to prove along the line of the above process that the final density operator now is given by

$$\rho_f = \frac{2}{N} \sum_{k=1}^{n} \varepsilon_k(P_k - M_k)I_{kz}$$

where the contribution of the $M_k$ part to the NMR signal of Eq.(17) comes from the phase-shift unitary operation $U_M(-\pi/2)$. The integer $M_k$ is given by

$$M_k = \sum_{l}^{M} a^l_k.$$  \hspace{1cm} (18)

Note that unlike the integer $P_k$ each integer $M_k$ is given in advance and can take any integer from $-N/2$ to $N/2$. Now the intensity of the NMR signal of the spin $k$ of the spin system in the ensemble is proportional to the subtraction $(P_k - M_k)$ of the two integers $P_k$ and $M_k$ instead of the single integer $P_k$. The subtraction $(P_k - M_k)$ can be positive, negative, or zero. Obviously, The subtraction $(G - M)$ is certainly an even number if there is zero-intensity NMR signal of the density operator $\rho_f$ of Eq.(17) for any arbitrary spin $k$ of the spin system in the ensemble. In the case the parity of the integer phase parameter $G$ can be determined directly from the subtraction $(G - M)$ since the integer $M$ is known, that is, $G$ is an even number if the integer $M$ is an even number, otherwise $G$ is an odd number. How to find the zero point of the subtraction $(P_k - M_k)$ with the above quantum algorithms? This is a classical one-dimensional search problem to find a zero point in mathematics.

At the first step the original quantum algorithm is run once, that is, making the oracle unitary operation of $U_o(\pi/2)$ on the initial density operator of Eq.(11), then adding a hard 90° pulse on the work qubits $I$ and a purge pulse on the ensemble, then applying a readout 90° pulse on the work qubits $I$ and recording the NMR signal of work qubits $I$ during decoupling the auxiliary qubits $S$ \[14\] by NMR phase-sensitive measurement \[5, 6\]. If one can find
that there is a zero-intensity NMR signal of any spin $k$ in the fast Fourier transform NMR spectroscopy of the recorded NMR signal, it can be certain that the integer phase parameter $G$ is an even number and the parity function $\text{par}(f) = +1$, otherwise one needs to run further the above modified quantum algorithm. Without losing generality, choose an arbitrary spin $k$ of the spin system in the ensemble with $P_k > 0$ (note that $N/2 \geq P_k \geq -N/2$), then a suitable phase-shift operation $U_M(-\pi/2)$ with $M_k = N/4$ is set up (if $P_k < 0$, $M_k = -N/4$). By running the modified quantum algorithm one can find either $(P_k - M_k) \neq 0$ or $(P_k + M_k) = 0$ from the fast Fourier transform NMR spectroscopy of the recorded NMR signal of Eq.(17). If $(P_k - M_k) = 0$ the parity problem is solved. If $(P_k - M_k) > 0$ a new phase-shift operation $U_M(-\pi/2)$ with $M_k = 3N/8$ is constructed, and if $(P_k - M_k) < 0$ another phase-shift operation $U_M(-\pi/2)$ with $M_k = N/8$ is built up. Then running the modified quantum algorithm again one can solve the parity problem if $(P_k - M_k) = 0$, otherwise construct again a new phase-shift unitary operation $U_M(-\pi/2)$, and then run the modified quantum algorithm again till one finds the zero point $(P_k - M_k) = 0$. Obviously, the above search process really uses the classical one-dimensional two partition method to search for a zero point. It needs $n$ times at most repeat running the quantum algorithm to find the zero point $(P_k - M_k) = 0$ (note that $N = 2^n$) by changing the number $M_k$. Therefore, one can solve efficiently the parity problem by repeating $n$ times at most to run the above quantum algorithm.

5. The explicit construction of the phase-shift unitary operation $U_M(-\pi/2)$

The phase-shift operations $U_M(-\pi/2)$ is a diagonal unitary operator and its effective Hamiltonian can be expanded in the longitudinal magnetization and spin order operator subspace [22]. It is the product of $M$ selective phase-shift operations $C_l(-\pi/2)$, as shown in Eq.(16). Without losing generality, one can set conveniently the index $k = 1$ and $M = |M_1|$ in Eq.(18), then for all $M$ indexes $l$ in the sum of Eq.(18) the unity numbers $\{a^l_1\}$ take the same value, i.e., $a^l_1 = +1$ ($M_1 > 0$), or $a^l_1 = -1$ ($M_1 < 0$). Then the phase-shift unitary operation $U_M(-\pi/2)$ in the unity-number vector representation $\{a^S_k\}$ may be expressed as, respectively,

$$
U_M(-\pi/2) = \exp[\text{i}\pi/2 \sum_1^M (\frac{1}{2}E_1 + I_{1z}) \otimes (\frac{1}{2}E_2 + a^l_2I_{2z}) \otimes \ldots \otimes (\frac{1}{2}E_n + a^l_nI_{nz})],
$$

(19a)
or

\[ U_M(-\pi/2) = \exp[i\pi/2 \sum_{l=1}^{M} (\frac{1}{2} E_1 - I_{1z}) \otimes (\frac{1}{2} E_2 + a_2 I_{2z}) \]
\[ \otimes ... \otimes (\frac{1}{2} E_n + a_n I_{nz})]. \quad (19b) \]

Without losing generality only \( U_M(-\pi/2) \) of Eq.(19a) with \( a_1^l = +1 \) for all index \( l \) is constructed explicitly below. One simple construction for the phase-shift unitary operations \( U_M(-\pi/2) \) is given explicitly by

\[ U_1(-\pi/2) = \exp[i\pi/2(\frac{1}{2} E_1 + I_{1z}) \otimes (\frac{1}{2} E_2 + I_{2z}) \otimes ... \]
\[ \otimes (\frac{1}{2} E_{n-1} + I_{n-1z}) \otimes (\frac{1}{2} E_n + I_{nz})], \]
\[ U_2(-\pi/2) = \exp[i\pi/2(\frac{1}{2} E_1 + I_{1z}) \otimes (\frac{1}{2} E_2 + I_{2z}) \otimes ... \otimes (\frac{1}{2} E_{n-1} + I_{n-1z})], \]
\[ U_3(-\pi/2) = \exp[i\pi/2(\frac{1}{2} E_1 + I_{1z}) \otimes (\frac{1}{2} E_2 + I_{2z}) \otimes ... \otimes (\frac{1}{2} E_{n-2} + I_{n-2z})] \]
\[ \times \exp[i\pi/2(\frac{1}{2} E_1 + I_{1z}) \otimes (\frac{1}{2} E_2 + I_{2z}) \otimes ... \otimes (\frac{1}{2} E_{n-1} + I_{n-1z})]. \]

\[ \ldots \]
\[ U_{2k}(-\pi/2) = \exp[i\pi/2(\frac{1}{2} E_1 + I_{1z}) \otimes (\frac{1}{2} E_2 + I_{2z}) \otimes ... \otimes (\frac{1}{2} E_{n-k} + I_{n-kz})] \]
\[ \ldots \]
\[ U_{N/2-1}(-\pi/2) = \exp[i\pi/2(\frac{1}{2} E_1 + I_{1z}) \otimes ... \otimes (\frac{1}{2} E_{n-1} + I_{n-1z})] \]
\[ \times \exp[-i\pi/2(\frac{1}{2} E_1 + I_{1z}) \otimes (\frac{1}{2} E_2 - I_{2z}) \otimes ... \otimes (\frac{1}{2} E_n - I_{nz})], \]
\[ U_{N/2}(-\pi/2) = \exp[i\pi/2(\frac{1}{2} E_1 + I_{1z})] \]

where the unity operator \( E_k \) is omitted without confusion in the direct product terms, for example, \((\frac{1}{2} E_1 + I_{1z}) \otimes ... \otimes (\frac{1}{2} E_{n-1} + I_{n-1z}) = (\frac{1}{2} E_1 + I_{1z}) \otimes ... \otimes (\frac{1}{2} E_{n-1} + I_{n-1z}) \otimes E_n). \) Obviously, besides the above construction there are a lot of other different constructions for the phase-shift operations which can be used to search for the zero point of \((P_k - M_k)\) in the present quantum algorithm. Because all these phase-shift unitary operations are not the oracle unitary operation and are given in advance one can construct their polynomial-time quantum circuits with the suitable interaction Hamiltonian of the spin system. In all the phase-shift unitary operations \( U_M(-\pi/2) \) the basic unitary operations are \( U_{2k}(-\pi/2) = C_0^{n-k}(-\pi/2) \) \((k = 0, 1, ..., n-1)\), where \( C_0^{n-k}(\theta) \) is a nonselective phase-shift operation in the spin subsystem with \( n - k \) qubits of the spin system with \( n \) qubits and is defined as \( C_0^{n-k}(\theta) = \exp(-i\theta D_0^{n-k}) \) (note that \( C_0^n(\theta) = C_0(\theta) \)) with the diagonal operator \( D_0^{n-k} = (\frac{1}{2} E_1 + I_{1z}) \otimes (\frac{1}{2} E_2 + I_{2z}) \otimes ... \otimes (\frac{1}{2} E_{n-k} + I_{n-kz}), \) \((k = 0, 1, ..., n-1)\). It is well known that the nonselective phase-shift operation \( C_0^{n-k}(\theta) \) \((\theta = \pi)\) is the basic unitary operation in the Grover algorithm [15] with \( 2^{n-k} \) dimensional search space. It is easy to prove that any phase-shift operation \( U_M(-\pi/2) \) \((1 \leq M \leq N/2 = 2^{n-1})\) can be expressed as the product of a polynomial number of the nonselective phase-shift operations.
in the single-qubit operations. As an example, the phase-shift operation \( U_M(-\pi/2) \) with \( M = 2^k + 2^l + 2^0 < 2^{k+1} \) can be expressed explicitly as

\[
U_M(-\pi/2) = C_0^{-k}(-\pi/2) \exp(-i\pi I_{n-kx}) C_0^{-l}(-\pi/2) \exp(-i\pi I_{n-lx}) \times C_0(-\pi/2) \exp(i\pi I_{n-lx}) \exp(i\pi I_{n-kx})
\]

In general case, the number \( M \) can be expressed by the binary representation as

\[
M = 2^k + b_{k-1}2^{k-1} + b_{k-2}2^{k-2} + \ldots + b_12^1 + b_02^0 < 2^{k+1}
\]

where \( b_l = 0, 1; l = 0, 1, \ldots, k - 1 \). Then the phase-shift operation \( U_M(-\pi/2) \) can be generally written as

\[
U_M(-\pi/2) = C_0^{-k}(-\pi/2) \exp(-i\pi I_{n-kx}) C_0^{-k+1}(-b_{k-1}\pi/2) \exp(-i\pi I_{n-k+1x}) \times C_0^{-k+2}(-b_{k-2}\pi/2) \exp(-i\pi I_{n-k+2x}) C_0^{-k+3}(-b_{k-3}\pi/2) \exp(-i\pi I_{n-k+3x}) \ldots \times C_0^{-1}(-b_1\pi/2) \exp(-i\pi I_{n-1x}) C_0(-b_0\pi/2) \exp(i\pi I_{n-1x}) \exp(i\pi I_{n-kx})
\]

Therefore, the phase-shift operation \( U_M(-\pi/2) \) can be expressed as the product of \((k+1)\) basic phase-shift operations \( C_0^{-k+l}(-\pi/2) \) \((l = 0, 1, \ldots, k; 0 \leq k \leq n - 1)\) and \(2k\) single-qubit unitary operations \( \exp(\pm i\pi I_{n-k+lx}) \) \((l = 0, 1, \ldots, k - 1)\) at most.

6. Discussion

It has showed in previous sections that the parity problem, one of the hardest problems in quantum and classical computations, can be solved efficiently on NMR quantum computers in polynomial time. It is based on the quantum parallelism principle in a quantum ensemble, selective decoherence manipulation, and the NMR phase-sensitive measurement. Because the parity function is a collective quantity one need not find all the function values so as to determine parity of the function on NMR quantum computers. In the paper the collective quantity \( G \) (see Eq.(8)) that reflects faithfully the parity problem is contained in the oracle unitary operations \( U_f \) and is used to determine efficiently the parity of function. The main drawback of the present quantum algorithm to solve the parity problem is that the detectable NMR signal reduces exponentially as the qubit number. To determine certainly the parity function with the present quantum algorithm it is required that the detectable NMR signal-to-noise ratio of the spin ensemble on an NMR machine must be as low as \( 2\varepsilon_k/N \), as can be seen in Eq.(14) or (17). These are similar to the basic characteristic feature of the conventional NMR quantum computers based on the effective pure states [9]. To implement really the present quantum algorithm one may still pay attention to the NMR dynamic
range problem on an NMR machine [5, 6]. This problem may be solved by using the spin ensemble of heteronuclear spin system. The present quantum algorithm is polynomial-time one, while those quantum algorithms running on the conventional quantum computers built up with the quantum system [1, 2] or based on the effective pure states [7, 8] cannot solve efficiently the parity problem and cannot outperform the classical algorithms. As an example, suppose that an NMR quantum computer with 30 qubits is available now [27]. Then to solve the parity problem with 30 qubits the present quantum algorithm needs \( \sim 30 \) calls of the oracle unitary operation \( U_o(\pi/2) \) or about 60 calls of the oracle unitary operation \( U_f \). However, it will need \( \sim 2^{30}/2 \) (\( \sim 5 \times 10^8 \)) calls of the oracle unitary operation \( U_f \) on the conventional quantum computer and \( 2^{30} \) (\( \sim 10^9 \)) calls of the oracle unitary operation \( U_f \) on a classical computer, respectively [1]. The difference of the call number of the oracle unitary operation is huge between the present quantum algorithm and the conventional or the classical one.

In comparison with the former scheme [14] to solve efficiently the parity problem based on the spectral labelling method [23] the present quantum algorithm is better one and more useful in practice. This is because the present quantum algorithm can be run on the spin ensemble of the linear molecules and does not required that the auxiliary qubits \( S \) are coupled with all the spins of the work qubits \( I \), and moreover, it can use the highly mix state of the spin ensemble instead of the effective pure state as the initial input state.

One could enhance the NMR signal of the final density operators of Eqs.(14) and (17) by running a quantum algorithm consisting of a polynomial number of the oracle unitary operations and nonselective unitary operations instead of the present quantum algorithm. However, the decoherence effect in a spin ensemble limits the possible call number of the oracle unitary operation in the quantum algorithm. Thus, there is a maximum call number of the oracle unitary operation in the quantum algorithm or a maximum run time \( T_{\text{max}} \) of the quantum algorithm in the spin ensemble due to the decoherence effect. The NMR signal will decrease simply but not be enhanced again as increasing the call number of the oracle unitary operation in the quantum algorithm if the call number is larger than the maximum one. This is because at that case running the quantum algorithm will take more time than \( T_{\text{max}} \), so that the decoherence effect becomes the dominant effect negatively upon the NMR signal. If the NMR signal is still too weak to be detected on an NMR machine when the quantum algorithm is run with the
maximum number calls of the oracle unitary operation, then other NMR signal enhancement methods such as the polarization transfer techniques, etc., [5, 6, 27-29] could be used to enhance the NMR signal and reach the same goal. Thus, here such NMR signal enhancement methods could be an effective scheme to overcome the decoherence effect on the quantum computation.

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