Efficient multiple-quantum transition processes in an n-qubit spin system

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Abstract

The whole Hilbert state space of an $n$-qubit spin system can be divided into $n + 1$ state subspaces according to the angular momentum theory of quantum mechanics. Here it is shown that any unknown state in such a state subspace, whose dimensional size is proportional to either a polynomial or exponential function of the qubit number $n$, can be transferred efficiently into a larger subspace with a dimensional size generally proportional to an exponential function of the qubit number by the multiple-quantum unitary transformation with a subspace-selective multiple-quantum unitary operator. The efficient quantum circuits for the subspace-selective multiple-quantum unitary operators are really constructed.

1. Multiple-quantum transition between state subspaces of the Hilbert space

Multiple-quantum transition processes [1] are closely related to the quantum computation [2, 3]. In a quantum system such as a coupled multiparticle two-level quantum system, e.g., an $n$-qubit spin system which may consist of $n$ coupled nuclei of spin $1/2$, quantum state transfer or transition between different states of the Hilbert space of the system generally consists of a variety of multiple-quantum transition processes except those noncoherent transition processes which are usually non-unitary processes [1]. A quantum search algorithm [4] running in a quantum system usually starts at an initial state such as a superposition, then performs a sequence of known unitary operations and the oracle unitary operation to convert the initial state into the marked state in a high efficiency, and finally makes a quantum-mechanically measure to output the marked state. A variety of quantum state transition or transfer from one state to another really occur in the quantum system during the quantum search process. The quantum search problem usually takes the whole Hilbert space of a quantum system as the search state space in which the unknown marked state is searched.
The computational complexity of the quantum search problem is closely related to the complexity of the multiple-quantum transition processes between different subspaces of the Hilbert space of the \( n \)–qubit spin system. The quantum state transition or transfer generally could not be efficient for an unknown state, e.g., the marked state in the quantum search problem from a state subspace of the Hilbert space whose dimensional size is proportional to an exponential function of qubit number \( n \) of the system into a smaller state subspace whose dimensional size increases polynomially as the qubit number, because a quantum state in a known subspace with a polynomial dimensional size can be determined in polynomial time. The multiple-quantum unitary transformation has been used to help design of quantum circuit [5] and quantum algorithms in quantum computation [2, 3]. The multiple-quantum spectra could be used to output results of quantum computation [3]. Using multiple-quantum unitary transformation the quantum search space of the quantum search problem [4] could be reduced from the whole Hilbert space of the \( n \)–qubit spin system to its largest subspace whose dimensional size is still much smaller than that of the whole Hilbert space, and hence this reduction could speed up the quantum search process. The more important is that the multiple-quantum unitary transformation provides a useful method to manipulate quantum state transition or transfer from a state to another or from a subspace to another in the Hilbert space in quantum computation.

The Hilbert space of an \( n \)–qubit spin system has a dimensional size \( 2^n \) which increases exponentially as the qubit number \( n \). It has \( 2^n \) conventional computational bases that can be used to represent \( 2^n \) numbers or elements in quantum computation. This is a large search space in the quantum search problem. The quantum search space will be reduced if the whole Hilbert space can be divided into small subspaces. In quantum computation this subspace reduction for the Hilbert space has been proposed to help design for the quantum search algorithm [2, 6]. There are a number of symmetric property of a quantum system to achieve the decomposition for its Hilbert space. The important one is the rotation symmetry in space of a quantum system [7-10]. The rotation symmetry in spin space of an \( n \)–qubit spin system which consists of \( n \) spins\( \frac{1}{2} \) may be used to guide the decomposition for the Hilbert space into its small subspaces. The angular momentum theory of quantum mechanics gives a detailed description for the rotation symmetry in space of a quantum system [7-10], and according to the angular momentum theory the whole Hilbert space of the \( n \)–qubit spin system may
be divided into \((n + 1)\) state subspaces, and each of which may be formed from the complete set of the eigenstates \(\{|\Psi_M\rangle\}\) of the total magnetic quantum operator \(I_z = \sum_{k=1}^{n} I_{kz}\) with a common eigenvalue \(M\) which satisfy the eigen-equation:

\[
I_z |\Psi_M\rangle = M |\Psi_M\rangle, \quad (\hbar = 1).
\]

The total magnetic quantum number (or the eigenvalue) \(M\) has \((n + 1)\) different values and can take \(n/2, n/2 - 1, \ldots, -n/2, -n/2\) for the \(n\)-qubit spin system. Each value of the quantum number \(M\) remarks a state subspace. The state subspace with the total magnetic quantum number \(M = n/2 - k\) is denoted as \(S(M = n/2 - k)\) or simply as \(S_{zq}(k)\) with \(k = 0, 1, \ldots, n\). Since all the states in a subspace take the same value of the total magnetic quantum number there is not a change for the value of the total magnetic quantum number in quantum transition between different states within the subspace and hence the quantum transition is a zero–quantum transition. A quantum state transition from a subspace to another is a nonzero-order quantum transition since the total magnetic quantum number value is changed when a state is transferred from a subspace into another. According to the angular momentum theory the dimensional size for the subspace \(S_{zq}(k)\) with \(k = 0, 1, \ldots, n\) is given by \(\binom{n}{k}\) for the \(n\)-qubit spin system, which is denoted as \(d(M = n/2 - k)\) or simply as \(d(k)\). Among the \((n + 1)\) subspaces the two smallest subspaces are \(S_{zq}(0)\) and \(S_{zq}(n)\), whose dimension is one. The next smallest subspaces are \(S_{zq}(1)\) and \(S_{zq}(n - 1)\) which have the same dimensional size \(n\). For a spin system with an even qubit number \(n\) the largest subspace is \(S_{zq}(n/2)\) and its dimensional size is \(d(n/2) = n!/[((n/2)!)^2]\). For a spin system with an odd qubit number the two largest subspaces are \(S_{zq}((n - 1)/2)\) and \(S_{zq}((n + 1)/2)\), respectively. Both the two subspaces have the same dimensional size equal \(d((n - 1)/2) = n!/[((n - 1)/2)!(n + 1)/2)]\). For a large \(n\) the number \(d(n/2) \approx d((n - 1)/2) \approx 2^n/\sqrt{\pi n/2}\) by the Starling’s formula. Therefore, the dimensional size for the largest subspace increases exponentially as the qubit number \(n\). Since any computational base of the Hilbert space of the spin system can be only in one of these \((n + 1)\) subspaces the quantum search space now may be limited to such a subspace in which the marked state is. When the marked state is in those smallest subspaces such as \(S_{zq}(0), S_{zq}(1), S_{zq}(2), \ldots\), whose dimensional size increases polynomially as the qubit number, it may be found in polynomial time. However, if the marked state is in the largest subspaces then it can be found by the
Grover quantum search algorithm [4] but this need take an exponential time proportional to $\sqrt{d(n/2)}$. Therefore, this shows indirectly that an unknown state usually could not be transferred efficiently from one large subspace whose dimensional size increases exponentially as the qubit number into a small subspace with a dimensional size proportional to a polynomial function of the qubit number. Actually, this quantum-state transfer is closely related to the computational complexity of the quantum search problem [4], that is, the quantum-state transfer is as hard as the latter one. However, the inverse quantum-state transfer process could be efficient, that is, an unknown state in a small subspace whose dimensional size may be proportional to an exponential or polynomial function of the qubit number could be efficiently transferred into a larger subspace by a multiple-quantum unitary transformation. These quantum-state transfer processes involve in quantum-state multiple-quantum transitions between different subspaces. It seems to see clearly that the quantum-state transfer could be efficient if an unknown state is initially in those smallest subspaces such as $S_{2q}(1)$, $S_{2q}(2)$, etc. However, it is not yet clear whether the quantum-state transfer is efficient or not if an unknown state is initially in those small subspaces whose dimensional size is also proportional to an exponential function of the qubit number. In the following a subspace-selective multiple-quantum unitary operator is constructed that transfers completely an unknown state from a subspace into a larger subspace of the Hilbert space.

Suppose that an unknown state $|\Psi_s\rangle$ is in a state subspace $S(M_s)$ and needs to be transferred to a larger subspace $S(M_s+p)$ by a multiple-quantum unitary transformation. The state $|\Psi_s\rangle$ can be expanded conveniently in terms of the usual computational basis $\{|\varphi_k(M_s)\rangle\}$ of the subspace $S(M_s)$:

$$
|\Psi_s\rangle = \sum_{k=0}^{d(M_s)-1} a_{sk} |\varphi_k(M_s)\rangle.
$$

If there is a $p$—quantum unitary operator that can convert simultaneously all the computational bases $\{|\varphi_k(M_s)\rangle\}$ in the unknown state $|\Psi_s\rangle$ from the subspace $S(M_s)$ into the subspace $S(M_s+p)$ then this $p$—quantum unitary operator also can convert the unknown state $|\Psi_s\rangle$ (2) from the subspace $S(M_s)$ into the subspace $S(M_s+p)$. It is possible to construct such a $p$—quantum unitary operator. Now dimensional sizes for the subspaces $S(M_s)$ and $S(M_s+p)$ are $d(M_s)$ and $d(M_s+p)$, respectively, and hence there are $d(M_s)$ and $d(M_s+p)$ computational bases in the subspaces $S(M_s)$
and $S(M_s + p)$, respectively. By using the computational bases of the two subspaces one can generate a subspace-selective $p-$quantum unitary operator that converts the unknown state $|\Psi_s\rangle$ from the subspace $S(M_s)$ into $S(M_s + p)$. Because $d(M_s + p)$ is greater than $d(M_s)$ one can choose properly any $d(M_s)$ bases among the $d(M_s + p)$ bases of the subspace $S(M_s + p)$. By combining these $d(M_s)$ computational bases from the subspace $S(M_s + p)$ with all the $d(M_s)$ computational bases of the subspace $S(M_s)$ one can build up $d(M_s)$ state-selective $p-$quantum Hermitian operators. For every pair of the computational bases $|\varphi_k(M_s)\rangle$ of the subspace $S(M_s)$ and $|\varphi_k(M_s + p)\rangle$ of the subspace $S(M_s + p)$ a state-selective $p-$quantum Hermitian operator is built up:

$$Q_{psk} = \frac{1}{2}(|\varphi_k(M_s)\rangle\langle\varphi_k(M_s + p)| + |\varphi_k(M_s + p)\rangle\langle\varphi_k(M_s)|).$$ (3)

Then the corresponding state-selective $p-$quantum unitary operator is generated from the Hermitian operator $Q_{psk}$ by

$$U_{psk}(\theta) = \exp(-i\theta Q_{psk}).$$ (4)

This state-selective $p-$quantum unitary operator is only applied to both the two states $|\varphi_k(M_s)\rangle$ of the subspace $S(M_s)$ and $|\varphi_k(M_s + p)\rangle$ of the subspace $S(M_s + p)$. There are $d(M_s)$ such state-selective $p-$quantum unitary operators. All these state-selective $p-$quantum unitary operators are commutable with each other because all the computational bases are orthogonal to each other. Then by multiplying all these $d(M_s)$ state-selective $p-$quantum unitary operators a subspace-selective $p-$order quantum unitary operator is obtained:

$$U_{ps}(\theta) = \prod_{k=0}^{d(M_s) - 1} U_{psk}(\theta) = \exp(-i\theta \sum_{k=0}^{d(M_s) - 1} Q_{psk}).$$ (5)

This $p-$quantum unitary operator is selectively applied to both the two subspaces $S(M_s)$ and $S(M_s + p)$. Since the dimensional size $d(M_s)$ of the subspace $S(M_s)$ may increase exponentially as the qubit number the unitary operator $U_{ps}(\theta)$ (5) may contain exponentially many state-selective $p-$quantum unitary operators (4). First it can be proved that the basis state $|\varphi_k(M_s)\rangle$ of the subspace $S(M_s)$ can be converted completely into the basis state $|\varphi_k(M_s + p)\rangle$ of the subspace $S(M_s + p)$ by the state-selective $p-$quantum unitary operator.
$U_{psk}(\theta)$. By expanding the unitary operator $U_{psk}(\theta)$ (4):

$$U_{psk}(\theta) = E + (-1 + \cos \frac{1}{2}\theta) (|\varphi_k(M_s)\rangle\langle\varphi_k(M_s)| + |\varphi_k(M_s + p)\rangle\langle\varphi_k(M_s + p)|) - 2Q_{psk} \sin \frac{1}{2}\theta$$

(6)

and using the orthogonormal condition for the usual computational bases one easily obtains

$$U_{psk}(\pi)|\varphi_{s'}(M_s)\rangle = \begin{cases} -i|\varphi_{s'}(M_s + p)\rangle, & \text{if } s' = k \\ |\varphi_{s'}(M_s)\rangle, & \text{if } s' \neq k \end{cases}.$$  

(7)

Therefore, the basis state $|\varphi_k(M_s)\rangle$ is transferred completely to the basis state $|\varphi_k(M_s + p)\rangle$ in addition to a phase factor $-i$ by the $p$-quantum unitary operator $U_{psk}(\pi)$. However, any other basis state of the subspace $S(M_s)$ keeps unchanged under the $p$-quantum unitary operator. This result can be further used to prove that any computational basis state $|\varphi_{s'}(M_s)\rangle$ of the subspace $S(M_s)$ can be converted completely into the basis state $|\varphi_{s'}(M_s + p)\rangle$ of the subspace $S(M_s + p)$ by the subspace-selective $p$-quantum unitary operator $U_{ps}(\pi)$ in (5). Because all the state-selective $p$-quantum unitary operators $Q_{psk}$ ($k = 0, 1, ..., d(M_s) - 1$) are commutative to each other one therefore has for any basis state $|\varphi_{s'}(M_s)\rangle$ of the subspace $S(M_s)$, by using (7),

$$U_{ps}(\pi)|\varphi_{s'}(M_s)\rangle = \prod_{k=0}^{d(M_s) - 1} \exp(-i\pi Q_{psk})|\varphi_{s'}(M_s)\rangle$$

$$= \exp(-i\pi Q_{ps's'})|\varphi_{s'}(M_s)\rangle$$

$$= -i|\varphi_{s'}(M_s + p)\rangle.$$  

(8)

Thus, the basis state $|\varphi_{s'}(M_s)\rangle$ is completely transferred into the basis state $|\varphi_{s'}(M_s + p)\rangle$ of the subspace $S(M_s + p)$ in addition to a total phase factor $-i$ by the $p$-quantum unitary operator $U_{ps}(\pi)$. This also indicates that all the basis states of the subspace $S(M_s)$ in the unknown state $|\Psi_s\rangle$ (2) can be simultaneously converted completely into the subspace $S(M_s + p)$ by the $p$-quantum unitary operator $U_{ps}(\pi)$. Then an arbitrary state of the subspace $S(M_s)$ also including $|\Psi_s\rangle$ with the expansion (2) can be also transferred completely into the subspace $S(M_s + p)$ by the $p$-quantum unitary operator $U_{ps}(\pi)$. 

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Generally, it is hard to construct an efficient subspace-selective multiple-quantum unitary operator that applies selectively on both two subspaces with exponentially many basis states. But since the larger subspace $S(M_s + p)$ has a larger dimensional size than the subspace $S(M_s)$ then it could be possible to construct such an efficient subspace-selective multiple-quantum unitary operator as $U_{ps}(\theta)$ (5) by suitably choosing the $d(M_s)$ bases $\{|\varphi_k(M_s + p)\rangle\}$ among all the $d(M_s + p)$ ($\geq d(M_s)$) computational bases of the subspace $S(M_s + p)$. An important subspace-selective $p$-quantum unitary operator of (5) is related to both a small subspace $S_{sq}(k)$ ($k \neq n/2$) and the largest subspace $S_{sq}(n/2)$ of the Hilbert space of an $n$-qubit spin system. If the marked state in the quantum search problem belongs to a state subspace $S_{sq}(k)$ ($k \neq n/2$) then using the known $p$-quantum unitary operator $U_{ps}(\pi)$ one may transfer efficiently it from the subspace $S_{sq}(k)$ into the largest subspace $S_{sq}(n/2)$. This really reduces the whole Hilbert space to its largest subspace $S_{sq}(n/2)$ as the search space of the quantum search problem. Below it is shown how an efficient quantum circuit for the subspace-selective $p$-quantum unitary operator (5) can be constructed in an $n$-qubit spin system.

2. The basic unitary operations

The basic unitary operations $U(\theta)$ used to build up the subspace-selective multiple-quantum unitary operators (5) may be generated from the Hermitian product operators $Q$ by the exponential mapping: $U(\theta) = \exp(-i\theta Q)$. The Hermitian product operators are the tension product operators of single-spin operators in an $n$-qubit spin system and generally written as $Q = H_1 \otimes H_2 \otimes ... \otimes H_n$. The Hermitian operator $H_k$ is the single-spin operator of the $k$th spin of the spin system and can be generally expressed as a linear combination of the single-spin magnetization operators $I_{kx}, I_{ky},$ and $I_{kz}$ as well as the unity operator $E_k$: $H_k = \alpha_{k0}E_k + \alpha_{kx}I_{kx} + \alpha_{ky}I_{ky} + \alpha_{kz}I_{kz}$, while the single-spin magnetization operators are related to Pauli's spin operators $\sigma_{k\mu}$ by $I_{k\mu} = \frac{1}{2} \sigma_{k\mu}$ ($\mu = x, y, z$). Every single-spin operator $H_k$ can be diagonalized: $\tilde{H}_k = U_k H_k U_k^+$, and its diagonal operator is given generally by $\tilde{H}_k = \alpha_k(\frac{1}{2}E_k + I_{kz}) + \beta_k(\frac{1}{2}E_k - I_{kz})$. Denote $\tilde{Q}$ as the diagonal operator of the product operator $Q$. Then the diagonal operator is generally written as $\tilde{Q} = \tilde{H}_1 \otimes \tilde{H}_2 \otimes ... \otimes \tilde{H}_n$. The complete operator set for the diagonal operators $\tilde{Q}$ forms the $LOMSO$ operator subspace [11]. The complete ba-
sis operator set for the LOMSO operator subspace usually may be chosen conveniently as the longitudinal magnetization and spin order operator set [11]:

\[ \bar{Q}_A = \{ E, I_{kz}, 2I_{kz}I_{lz}, 4I_{kz}I_{lz}I_{mz}, \ldots, 2^{n-1}I_{kz}I_{lz}I_{mz} \ldots I_{nz} \}. \]

In addition to the longitudinal magnetization and spin order operator set there are also other equivalent complete basis operator sets, of which a particularly important basis operator set is given by [2]

\[ \bar{Q}_B = \{ E, D_{l}^{k_1k_2}, \ldots, D_{l}^{k_1k_2 \ldots k_n} \}, \]

where the diagonal operator \( D_{l}^{k_1k_2 \ldots k_m} (m = 1, 2, \ldots, n; l = 0, 1, \ldots, 2^m - 1) \) is defined by

\[
D_{l}^{k_1k_2 \ldots k_m} = \left( \frac{1}{2} E_{k_1} + a_{k_1}^l I_{k_1z} \right) \otimes \left( \frac{1}{2} E_{k_2} + a_{k_2}^l I_{k_2z} \right) \otimes \ldots \otimes \left( \frac{1}{2} E_{k_m} + a_{k_m}^l I_{k_mz} \right), \tag{9}
\]

where the indices \( k_1, k_2, \ldots, k_n \) and \( k, l, m, \ldots, \) are series number of spins in the spin system and usually are ordered: 1 \( \leq \) \( k_1 < k_2 < \ldots < k_n \leq n \), 1 \( \leq k < l < \ldots \leq n \); \( \{ a_{k}^l \} \) is a quantum-state unit-number vector, \( a_{k}^l = \pm 1 \); and all the unity operator components \( \{ E_{k} \} \) in the product operators are omitted for convenience, for example, the full expressions for the product operators \( 2I_{kz}I_{lz} \) and \( D_{l}^{k_1k_2} \) should be given respectively by

\[
2I_{kz}I_{lz} \equiv 2E_1 \otimes \ldots \otimes E_{k-1} \otimes I_{kz} \otimes E_{k+1} \otimes \ldots
\]

\[
\otimes E_{l-1} \otimes I_{lz} \otimes E_{l+1} \otimes \ldots \otimes E_{n},
\]

\[
D_{l}^{k_1k_2} \equiv E_1 \otimes \ldots \otimes E_{k_1-1} \otimes \left( \frac{1}{2} E_{k_1} + a_{k_1}^l I_{k_1z} \right) \otimes E_{k_1+1} \otimes \ldots
\]

\[
\otimes E_{k_2-1} \otimes \left( \frac{1}{2} E_{k_2} + a_{k_2}^l I_{k_2z} \right) \otimes E_{k_2+1} \otimes \ldots \otimes E_{n}.
\]

In particular, denote that the diagonal operator \( D_{m,l} \equiv D_{l}^{12 \ldots m} = \bigotimes_{k=1}^{m} \left( \frac{1}{2} E_{k} + a_{k}^l I_{kz} \right) (m = 1, 2, \ldots, n; l = 0, 1, \ldots, 2^m - 1) \), and there is a simple denotation \( D_{l} \equiv D_{n,l} \) used also in previous papers [2, 6]. The diagonal operator \( D_{m,l} \) is called the quantum-state diagonal operator since a conventional computational basis state of an \( m \)-qubit spin system can be characterized completely by the quantum-state unit-number vector \( \{ a_{k}^l \} \) or equivalently by the diagonal operator \( D_{m,l} \) [2].

It is clear that both the basis operator sets \( \bar{Q}_A \) and \( \bar{Q}_B \) are equivalent to each other. By expanding the diagonal operator \( D_{l}^{k_1k_2 \ldots k_m} \) (9) it can be seen that the operator is a linear combination of the product operators of the set \( \bar{Q}_A \). On the other hand, using the operator identity: \( 2I_{kz} = \left( \frac{1}{2} E_{k} + I_{kz} \right) - \left( \frac{1}{2} E_{k} - I_{kz} \right) \)
$(\frac{1}{2}E_k - I_{kz})$ every product operator in the set $\tilde{Q}_A$ also can be expressed as a linear combination of the basis operators of the set $\tilde{Q}_B$.

It is known that elementary propagators built up with the basis operators of the operator set $\tilde{Q}_A$ can be implemented efficiently. For the elementary propagators there is a simple recursive relation for decomposing a multi-body elementary propagator built up with a multi-body interaction basis operator, e.g., $2^{m-1}I_{k_1z}I_{k_2z}...I_{k_mz}$, into a sequence of one- and two-body elementary propagators. Generally, the elementary propagator $R_{k_1k_2...k_m}(\theta) = \exp(-i\theta 2^{m-1}I_{k_1z}I_{k_2z}...I_{k_mz})$ ($2 < m \leq n$) can be simply decomposed as [5]

$$ R_{k_1k_2...k_m}(\theta) = \exp(-i\frac{\pi}{2}I_{k_{m-1}z}) \exp(-i\pi I_{k_{m-1}z}I_{k_{m}z}) \times \exp(-i\frac{\pi}{2}I_{k_{m-1}y}) \exp(-i\theta 2^{m-2}I_{k_1z}I_{k_2z}...I_{k_{m-1}z}) \times \exp(i\frac{\pi}{2}I_{k_{m-1}y}) \exp(i\pi I_{k_{m-1}z}I_{k_{m}z}) \exp(i\frac{\pi}{2}I_{k_{m-1}x}). $$

(10)

This recursive relation assures that any elementary propagator built up with the basis operator of the operator set $\tilde{Q}_A$ can be efficiently decomposed into a sequence of one- and two-qubit quantum gates.

The basic unitary operations built up with the basis operators of the operator set $\tilde{Q}_B$ also can be implemented efficiently. It is based on the fact that the selective rotation operation applying only to a given state of any $m$–qubit subsystem ($1 \leq m \leq n$) of an $n$–qubit spin system can be implemented efficiently. It is known that the selective rotation operation $C_0(\theta) = \exp(-i\theta D_0)$ built up with the basis operator $D_0 = \bigotimes_{k=1}^{n} (\frac{1}{2}E_k + I_{kz})$ of the operator set $\tilde{Q}_B$ can be performed efficiently in an $n$–qubit spin system [2, 4]. This is an $n$–qubit selective rotation operation applying only to the known state $|0_1\rangle|0_2\rangle...|0_n\rangle$ of the $n$–qubit spin system. Generally, an $m$–qubit selective rotation operation with $1 \leq m \leq n$ can be also performed efficiently in the $n$–qubit spin system. This $m$–qubit selective rotation operation is only applied to the known state $|0_1\rangle|0_2\rangle...|0_m\rangle$ of the $m$–qubit subsystem consisting of the first $m$ spins of the $n$–qubit spin system when it is applied to any basis state $|0_1\rangle|0_2\rangle...|0_m\rangle|\varphi_{m+1}\rangle...|\varphi_{n}\rangle$ of the $n$–qubit spin system ($|\varphi_{m+1\rangle}, |\varphi_{m+2}\rangle, ..., |\varphi_{n}\rangle$ take $|0\rangle$ or $|1\rangle$). It is defined by [2]

$$ C_{m,0}(\theta) = \exp(-i\theta D_{m,0}). $$

(11)
There is a simple denotation: \( C_l(\theta) = C_{n,l}(\theta) \) also used in previous papers [2, 6].

The efficient implementation for the \( m \)-qubit selective rotation operation \( C_{m,0}(\theta) \) may use conveniently the reversible AND operations and conditional phase shift operations. The classical AND operation is really irreversible and it needs to be changed to the reversible one by the Bennett’s method [12] when it is used to construct these selective rotation operations.

More generally, any \( m \)-qubit selective rotation operation \( C_{k_1 k_2 \ldots k_m}(\theta) \) of any \( m \)-qubit subsystem \((1 \leq m \leq n)\) of the \( n \)-qubit spin system also can be performed efficiently,

\[
C_{k_1 k_2 \ldots k_m}(\theta) = \exp(-i\theta D_{k_1 k_2 \ldots k_m}), \tag{12}
\]

where the diagonal operator \( D_{k_1 k_2 \ldots k_m} \) \((1 \leq m \leq n, 0 \leq l \leq 2^m - 1)\) is a basis operator of the operator set \( \hat{Q}_B \) given by definition (9). In particular, \( C_{m,0}(\theta) \equiv C_{12 \ldots m}(\theta) \). The \( m \)-qubit selective rotation operation \( C_{0 k_1 k_2 \ldots k_m}(\theta) \) is only applied to any state \( |0\rangle_{k_1} \ldots |0\rangle_{k_2} \ldots |0\rangle_{k_m} \) with the known state \( |0\rangle \) of the \( k_1 \)th, \( k_2 \)th, ..., \( k_m \)th spins of the \( n \)-qubit spin system. The diagonal operator \( D_{0 k_1 k_2 \ldots k_m} \) can be really converted efficiently into the diagonal operator \( D_{m,0} \). This can be achieved with the help of the zero-quantum unitary transformation:

\[
I_k = V_{kl}(\pi)I_l V_{kl}(\pi)^+, \tag{13}
\]

where the zero-quantum unitary operator is given by

\[
V_{kl}(\theta) = \exp[-i\theta \frac{1}{2}(2I_{kx}I_{ly} - 2I_{ky}I_{lx})],
\]

which can be decomposed into a sequence of two two-qubit quantum gates:

\[
V_{kl}(\theta) = \exp(-i\theta I_{kx}I_{ly}) \exp(i\theta I_{ky}I_{lx}). \tag{14}
\]

Assume that the indices in the diagonal operator \( D_{0 k_1 k_2 \ldots k_m} \) satisfy \( 1 \leq k_1 < k_2 < \ldots < k_m \leq n \). If the index \( k_1 \neq 1 \) then making the zero-quantum unitary transformation (13) with the zero-quantum unitary operator \( V_{kl}(\pi) \) (14) with the indices \( k = 1 \) and \( l = k_1 \) on the diagonal operator \( D_{0 k_1 k_2 \ldots k_m} \) the operator \( D_{0 k_1 k_2 \ldots k_m} \) is converted into \( D_{1 k_2 \ldots k_m} \), and if \( k_1 = 1 \) then \( D_{0 k_1 k_2 \ldots k_m} = D_{1 k_2 \ldots k_m} \) and no unitary transformation is needed to apply on the operator \( D_{0 k_1 k_2 \ldots k_m} \). In a similar way, if the index \( k_2 \neq 2 \) then \( D_{1 k_2 \ldots k_m} \) is converted into \( D_{0 1 k_3 \ldots k_m} \) by \( V_{kl}(\pi) \) with the indices \( k = 2 \) and \( l = k_2 \).
By making the zero-quantum unitary transformation (13) on the diagonal operator \( D_0^{k_1k_2...k_m} \) at most \( m \) times one can convert completely the diagonal operator \( D_0^{k_1k_2...k_m} \) into the diagonal operator \( D_0^{12...m} (\equiv D_{m,0}) \). Then the selective rotation operations \( C_0^{k_1k_2...k_m}(\theta) \) (12) can be implemented efficiently since \( C_{m,0}(\theta) \) can be performed efficiently. Finally, using \( m \) pulses \( \exp(-i\pi I_{k_x}) \) or \( \exp(-i\pi I_{k_y}) \) at most one can convert the diagonal operator \( D_{m,l} \) into \( D_{m,0} \) and \( D_l^{k_1k_2...k_m} \) into \( D_0^{k_1k_2...k_m} \) for any index \( l \neq 0 \). This is based on the fact that \( \frac{1}{2}E_k + I_{k_z} \equiv \exp(-i\pi I_{k_{\mu}})(\frac{1}{2}E_k - I_{k_z})\exp(i\pi I_{k_{\mu}}) \) \( (\mu = x, y) \). Then any \( m \)-qubit selective rotation operation \( C_l^{k_1k_2...k_m}(\theta) \) (12) can be performed efficiently.

Therefore, the basic quantum gates used to construct quantum circuits for multiple-quantum unitary operators include three types:

(i) the \( m \)-qubit selective rotation operations: \( C_{m,0}(\theta) \) \( (m = 1, 2, \ldots, n) \),
(ii) the two-qubit quantum gates: \( \exp(-iJ_{kl}2I_{k_2}I_{l_2}) \) \( (k, l = 1, 2, \ldots, n) \),
(iii) the single-qubit gates: \( \exp(-i\theta_{k_{\mu}}I_{k_{\mu}}) \) \( (\mu = x, y, z; k = 1, 2, \ldots, n) \).

Obviously, the three types of basic quantum gates form the universal quantum gate set in quantum computation.

Once the elementary propagators formed from the basis operators of the product operator sets \( Q_A \) and \( Q_B \) can be implemented efficiently then these basic unitary operations \( U_\beta(\theta) = \exp(-i\theta Q_\beta) \) \( (\beta = a, b, c) \) built up with the following three types of the basic product operators also can be efficiently implemented:

(i) \( Q_a = 2^{l-1}I_{k_1\mu_1} \bigotimes I_{k_2\mu_2} \bigotimes \ldots \bigotimes I_{k_l\mu_l} \bigotimes E_{k_{l+1}} \bigotimes \ldots \bigotimes E_{k_n} \);
(ii) \( Q_b = (\frac{1}{2}E_{k_l} + a^I_{k_l}I_{k_1\mu_1}) \bigotimes (\frac{1}{2}E_{k_2} + a^I_{k_2}I_{k_2\mu_2}) \bigotimes \ldots \bigotimes (\frac{1}{2}E_{k_l} + a^I_{k_l}I_{k_l\mu_l}) \bigotimes E_{k_{l+1}} \bigotimes \ldots \bigotimes E_{k_n} \);
(iii) \( Q_c = 2^{l-1}I_{k_1\mu_1} \bigotimes \ldots \bigotimes I_{k_l\mu_l} \bigotimes (\frac{1}{2}E_{k_{l+1}} + a^I_{k_{l+1}}I_{k_{l+1}\mu_{l+1}}) \bigotimes \ldots \bigotimes (\frac{1}{2}E_{k_n} + a^I_{k_n}I_{k_n\mu_n}) \bigotimes E_{k_{n+1}} \bigotimes \ldots \bigotimes E_{k_n} \),

where \( \mu_{\alpha} = x, y, z \) \( (\alpha = 1, 2, \ldots, n) \). This is because each of these product operators always can be efficiently converted into a basis operator or a sum of two basis operators of the product operator sets \( Q_A \) and \( Q_B \) with the help of the recursive relation (10), the zero-quantum unitary transformation (13), and the single-spin rotation operations: \( \exp(-i\theta I_{k_{\mu}}) \) \( (\mu = x, y, z) \). As an example, suppose that a product operator \( Q_c \) is given by

\[
Q_c = 2I_{1x} \bigotimes E_{2} \bigotimes (\frac{1}{2}E_3 + I_{3x}) \bigotimes I_{4z} \bigotimes (\frac{1}{2}E_5 - I_{5z}).
\]
Then it can be expressed as

\[ Q_c = R_0 \left[ (\frac{1}{2} E_1 + I_{1z}) \otimes E_2 \otimes (\frac{1}{2} E_3 + I_{3z}) \otimes E_4 \otimes (\frac{1}{2} E_5 + I_{5z}) - \frac{1}{2} E_1 \otimes E_2 \otimes (\frac{1}{2} E_3 + I_{3z}) \otimes E_4 \otimes (\frac{1}{2} E_5 + I_{5z}) \right] R_0^+ \]

where the unitary operator \( R_0 \) is determined by the recursive relation (10) and the single-spin rotation operations,

\[ R_0 = \exp(i\pi I_{1y}) \exp(i\pi I_{3y}) \exp(-i\pi I_{5x}) \times \exp(-i\pi I_{1x}) \exp(-i\pi I_{1z}I_{4z}) \exp(-i\pi I_{1y}). \]

If the zero-quantum unitary transformation (13) is further used then the unitary operator \( \exp(-i\theta Q_c) \) can be thoroughly decomposed as a sequence of the basic quantum gates:

\[ \exp(-i\theta Q_c) = R_0 V_{23}(\pi)^+ V_{35}(\pi)^+ C_{3,0}(\theta) V_{35}(\pi) V_{23}(\pi) \times V_{13}(\pi)^+ V_{25}(\pi)^+ C_{2,0}(\theta/2) V_{13}(\pi) V_{25}(\pi) R_0^+. \]

3. The quantum circuits for the subspace-selective multiple-quantum unitary operations

3.1 The Hermitian diagonal operators

Two types of Hermitian operators will be used to generate the multiple-quantum unitary operators (5). The first type simply consists of the \((n + 1)\) Hermitian diagonal operators \( \{g_0, g_1, g_2, ..., g_n\} \) for an \(n\)-qubit spin system. Each of the diagonal operators corresponds one-to-one to one state subspace \( S_{2q}(k) \). The diagonal operators are generated from the quantum-state diagonal operator set \( \{D_k\} \). Their definition is given below.

\[ g_0 = D_0, D_0 \in S_{2q}(0) \times S_{2q}(0), \]

or in the matrix representation the diagonal operator \( g_0 \) is written as

\[ g_0 = \begin{bmatrix} 1 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{bmatrix} \equiv \text{Diag}(1_0, 0_1, ..., 0_{N-1}); \]

12
\[
g_1 = \sum_k D_k, D_k \in S_{zq}(1) \times S_{zq}(1),
\]
\[
\begin{bmatrix}
0 & 1 & \cdots \\
1 & 0 & \cdots \\
\vdots & \vdots & \ddots
\end{bmatrix}
\]
or \[
g_1 = \begin{bmatrix}
0 & 1 & \cdots \\
1 & 0 & \cdots \\
\vdots & \vdots & \ddots
\end{bmatrix} \equiv \text{Diag}(0, 1, \ldots, 1_{L_1}, 0_{L_1}, \ldots, 0_{N-1}),
\]
l_1 = d(0) = 1, L_1 = l_1 + d(1) - 1;
\[
g_2 = \sum_k D_k, D_k \in S_{zq}(2) \times S_{zq}(2),
\]
or \[
g_2 = \text{Diag}(0, 1_{l_2}, \ldots, 1_{L_2}, 0_{L_2}, \ldots, 0_{N-1}),
\]
l_2 = d(0) + d(1), L_2 = l_2 + d(2) - 1;
\[
g_m = \sum_k D_k, D_k \in S_{zq}(m) \times S_{zq}(m),
\]
or \[
g_m = \text{Diag}(0, 1_{l_m}, \ldots, 1_{L_m}, 0_{L_m}, \ldots, 0_{N-1}),
\]
l_m = d(0) + d(1) + \ldots + d(m - 1), L_m = l_m + d(m) - 1;
\[
g_n = D_{N-1}, D_{N-1} \in S_{zq}(n) \times S_{zq}(n),
\]
or \[
g_n = \begin{bmatrix}
0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & 1
\end{bmatrix} \equiv \text{Diag}(0, 1, \ldots, 0_{N-2}, 1_{N-1}),
\]
where again \(d(m) = \binom{n}{m}\) is dimensional size of the subspace \(S_{zq}(m)\); \(l_m\) and \(L_m\) are diagonal-element indices in the matrix \(g_m\); and \(S_{zq}(m) \times S_{zq}(m)\) is the zero-quantum operator subspace corresponding to the subspace \(S_{zq}(m)\) whose basis operator set may be simply \(\{ |k\rangle \langle l|\} \) with any basis states \(|k\rangle, |l\rangle \in S_{zq}(m)\). This zero-quantum operator subspace also includes the diagonal operator \(g_m\). Obviously, the unitary rotation operation \(G_m(\theta) = \exp(-i\theta g_m)\) \((m = 0, 1, 2, \ldots, n)\) can be expressed as a sequence of the selective rotation
operations applied only on the states of the subspace $S_{zq}(m)$:

$$G_m(\theta) = \prod_{k=l_m}^{L_m} C_k(\theta)$$  \hspace{1cm} (15)

where $C_k(\theta) \equiv C_{n,k}(\theta) = \exp(-i\theta D_k)$ given by (11) with the diagonal operator $D_k \in S_{zq}(m) \times S_{zq}(m)$ is a selective rotation operation applied only to the computational base $|\varphi_k\rangle$ of the subspace $S_{zq}(m)$, where the computational base $|\varphi_k\rangle = \bigotimes_{i=1}^n (\frac{1}{2} T_i + a_i^k S_i)$, $T_i = |0_i\rangle + |1_i\rangle$ and $S_i = \frac{1}{2}(|0_i\rangle - |1_i\rangle)$ [2].

It can be seen from (15) that the rotation operation $G_m(\theta)$ of the subspace $S_{zq}(m) \times S_{zq}(m)$ with $m \sim n/2$ is an exponential sequence of the selective rotation operations with number $d(m)$. But it may be really simplified and its efficient quantum circuit may be built up with the elementary propagators $R_{k_1 k_2 \ldots k_m}(\theta)$ (10) and $C_{l_1 l_2 \ldots l_m}(\theta)$ (12).

The diagonal matrix $g_m$ has $d(m)$ and $(2^n - d(m))$ diagonal elements taking one and zero, respectively. The $(2^n - d(m))$ zero-diagonal elements are divided into two parts by the $d(m)$ one-diagonal elements, and numbers for the first part and the second are $l_m$ and $(2^n - d(m) - l_m)$, respectively. Note that $2^n = l_m + d(m) + (2^n - d(m) - l_m)$ is an even number. Then there are only two possibilities: (i) all the three numbers $l_m$, $d(m)$, and $(2^n - d(m) - l_m)$ are even or (ii) one of the three numbers must be even and the other two numbers are odd. For the first case that all the three numbers are even the diagonal operator $g_m$ can be reduced to the form

$$g_m \equiv \text{Diag}(0, \ldots, 0; 1_{l_m}, \ldots, 1_{L_m}; 0, \ldots, 0)$$

$$= \text{Diag}(0, \ldots, 0; 1_{l_m/2}, \ldots, 1_{L_m/2}; 0, \ldots, 0)_{2^{n-1} \times 2^{n-1}} \bigotimes E_n. $$

Now the new diagonal operator $\text{Diag}(0, \ldots, 0; 1_{l_m/2}, \ldots, 1_{L_m/2}; 0, \ldots, 0)_{2^{n-1} \times 2^{n-1}}$ is applied only to the subsystem with the first $n-1$ qubits of the $n$–qubit spin system. Its dimensional size is $2^{n-1} \times 2^{n-1}$, which is denoted in the subscript for convenience, instead of dimensional size $2^n \times 2^n$ of the original diagonal operator $g_m$. The number of the diagonal elements taking one in the operator $\text{Diag}(0, \ldots, 0; 1, \ldots, 1; 0, \ldots, 0)_{2^{n-1} \times 2^{n-1}}$ now is $d(m)/2$. The unitary operation $G_m(\theta)$ then is simplified (as defined),

$$G_m(\theta) = \exp[-i\theta \text{Diag}(0, \ldots, 0; 1_{l_m/2}, \ldots, 1_{L_m/2}; 0, \ldots, 0)_{2^{n-1} \times 2^{n-1}} \bigotimes E_n]$$

$$\equiv \exp[-i\theta \text{Diag}(0, \ldots, 0; 1_{l_m/2}, \ldots, 1_{L_m/2}; 0, \ldots, 0)_{2^{n-1} \times 2^{n-1}}].$$
Thus, the unitary operation $G_m(\theta)$ is really applied only to the subsystem with the first $n-1$ qubits of the $n$-qubit spin system and hence is reduced to a $(n-1)$-qubit rotation operation of the $(n-1)$-qubit spin subsystem. If now the rotation operation $G_m(\theta)$ is still expressed as a sequence of the selective rotation operation applied to the $(n-1)$-qubit subsystem then number of the selective rotation operations, i.e., $d(m)/2$, in the sequence is a half of the original one. Obviously, such a reduction can be further carried out.

It is slightly complicated for another case that only one number is even among the three numbers $l_m$, $d(m)$, and $(2^n - d(m) - l_m)$. In this case there are only three possible options:

(a) $l_m$ is an even number. Then $d(m)$ is an odd number. The diagonal operator $g_m$ can be simplified by

$$g_m = \text{Diag}(0, ..., 0; 1_{l_m/2}, ..., 1_{(l_{m-1})/2}; 0, ..., 0)2^{n-1} \times 2^{n-1} \bigotimes E_n + D_{L_m}$$

where the diagonal operator $D_{L_m} = \text{Diag}(0, ..., 0; 0_{l_m}, ..., 0_{l_{m-1}}, 1_{L_m}; 0, ..., 0)$, and the diagonal operator $\text{Diag}(0, ..., 0; 1_{l_m/2}, ..., 1_{(l_{m-1})/2}; 0, ..., 0)2^{n-1} \times 2^{n-1}$ has $(d(m) - 1)/2$ one-diagonal elements and is a $(n-1)$-qubit diagonal operator. Because all the diagonal operators are commutative to each other the corresponding unitary operation $G_m(\theta)$ is decomposed as

$$G_m(\theta) = C_{L_m}(\theta) \exp[-i \theta \text{Diag}(0, ..., 0; 1_{l_m/2}, ..., 1_{(l_{m-1})/2}; 0, ..., 0)2^{n-1} \times 2^{n-1}].$$

Therefore, the diagonal unitary operation $G_m(\theta)$ is decomposed into a product of an $n$-qubit selective rotation operation $C_{L_m}(\theta)$ and a $(n-1)$-qubit diagonal unitary operation of the $n$-qubit spin system.

(b) $d(m)$ is an even number. Then the diagonal operator $g_m$ is written as

$$g_m = D_{l_m} + D_{L_m} + \text{Diag}(0, ..., 0; 1_{(l_m+1)/2}, ..., 1_{(L_m-1)/2}; 0, ..., 0)2^{n-1} \times 2^{n-1} \bigotimes E_n.$$ 

The diagonal operator $\text{Diag}(0, ..., 0; 1_{(l_m+1)/2}, ..., 1_{(L_m-1)/2}; 0, ..., 0)2^{n-1} \times 2^{n-1}$ is a $(n-1)$-qubit diagonal operator with $(d(m) - 2)/2$ one-diagonal elements. The corresponding unitary operation $G_m(\theta)$ is expressed as

$$G_m(\theta) = C_{l_m}(\theta)C_{L_m}(\theta) \exp[-i \theta \text{Diag}(0, ..., 0; 1_{(l_m+1)/2}, ..., 1_{(L_m-1)/2}; 0, ..., 0)2^{n-1} \times 2^{n-1}].$$
This shows that the diagonal unitary operation $G_m(\theta)$ now is decomposed into a product of two $n$–qubit selective rotation operations $C_{t_m}(\theta)$ and $C_{L_m}(\theta)$ and a $(n – 1)$–qubit diagonal unitary operation.

(c) $(2^n – d(m) – l_m)$ is an even number. The diagonal operator $g_m$ is simplified by

$$g_m = D_{t_m} + Diag(0, ..., 0; 1_{(l_m+1)/2}; ..., 1_{L_m/2}; 0, ..., 0)_{2^n-1 \times 2^n-1} \otimes E_n.$$  

The diagonal operator $Diag(0, ..., 0; 1_{(l_m+1)/2}; ..., 1_{L_m/2}; 0, ..., 0)_{2^n-1 \times 2^n-1}$ now is a $(n – 1)$–qubit diagonal operator with $(d(m) – 1)/2$ one-diagonal elements. The corresponding unitary operation $G_m(\theta)$ can be decomposed as

$$G_m(\theta) = C_{t_m}(\theta) \exp[-i\theta Diag(0, ..., 0; 1_{(l_m+1)/2}; ..., 1_{L_m/2}; 0, ..., 0)_{2^n-1 \times 2^n-1}].$$

Thus, the diagonal unitary operation $G_m(\theta)$ now is decomposed into a product of one $n$–qubit selective rotation operation $C_{t_m}(\theta)$ and another $(n – 1)$–qubit diagonal unitary operation.

As a summary, in either case the $n$–qubit diagonal unitary operator $G_m(\theta)$ can be reduced to a product of a $(n – 1)$–qubit diagonal unitary operator and two $n$–qubit selective rotation operators at most.

The $(n – 1)$–qubit rotation operation $\exp[-i\theta Diag(0, ..., 0; 1, ..., 1; 0, ..., 0)_{2^n-1 \times 2^n-1}]$ can be further reduced to the $(n – 2)$–qubit rotation operation $\exp[-i\theta Diag(0, ..., 0; 1, ..., 1; 0, ..., 0)_{2^{n-2} \times 2^{n-2}}]$ which has around $d(m)/2^2$ one-diagonal elements, but this reduction may yield extra two $(n – 1)$–qubit selective rotation operations $C_{n-1,t_m}(\theta)$ (the index $t_m$ is dependent on $l_m$ and $L_m$) at most, so that the unitary operator $G_m(\theta)$ now is a product of a $(n – 2)$–qubit rotation operation and four $n$– and $(n – 1)$–qubit selective rotation operations at most. This reduction process can continue to the end when the diagonal operator $g_m$ is reduced to the final form

$$Diag(0, ..., 0; 1, 1; 0, ..., 0)_{2^n-k \times 2^n-k} \otimes E_{k+1} \otimes ... \otimes E_n$$  \hspace{1cm} (16)$$

or

$$Diag(0, ..., 0; 1; 0, ..., 0)_{2^n-k \times 2^n-k} \otimes E_{k+1} \otimes ... \otimes E_n,$$  \hspace{1cm} (17)$$

where $k$ satisfies $2^k \approx d(m)$ and is less than $n – 1$ because $d(m) < 2^{n-1}$ for $n > 2$. The first diagonal operator (16) can form two $(n – k)$–qubit selective rotation operations and the second (17) can generate only one $(n – k)$–qubit selective rotation operation. Since each reduction step can generate two
selective rotation operations \( C_{l,t,m}(\theta) \) at most the diagonal unitary operator \( G_m(\theta) \) can be expressed as a sequence of \( l \)-qubit selective rotation operations \( C_{l,t,m}(\theta) \) \((l = k, k + 1, \ldots, n)\) with a total number less than \( 2n \).

The same decomposition procedure as the above can be carried out for a general diagonal operator \( Diag(0, \ldots, 0_{l-1}; 1_l, \ldots, 1_{L}; 0_{L+1}, \ldots, 0_{N-1}) \) that may not be in only one zero-quantum operator subspace, e.g., \( S_{zq}(m) \times S_{zq}(m) \), and consequently the diagonal operator may be expressed as a sequence of \( l \)-qubit selective rotation operations \( C_{l,t,m}(\theta) \) \((l = k, k + 1, \ldots, n)\) with number less than \( 2^k \), where \( k \) satisfies \( 2^k \approx (L - l + 1) \) and is less than \( n \).

3.2 The Hermitian anti-diagonal operators

Another type of the Hermitian operators used to generate the subspace-selective multiple-quantum unitary operators are anti-diagonal Hermitian operators. They are a generalization of the product operator \( 2^{n-1}I_{1x}I_{2x}I_{nx} \) \([2, 6]\) and are defined in a matrix form by

\[
b_0 = \begin{bmatrix}
0 & 1 \\
0 & 1 & 0 \\
& & 0 \\
& 0 & \\
1 & 0 & \\
& & & &
\end{bmatrix},
b_1 = \begin{bmatrix}
0 & 1 & 0 \\
0 & 1 & 0 \\
& & 0 \\
& 0 & \\
1 & 0 & \\
& & & &
\end{bmatrix},
b_{-1} = \begin{bmatrix}
0 & \\
0 & 1 & 0 \\
& 0 & \\
& 0 & \\
& 1 & \\
& & & &
\end{bmatrix},
b_2 = \begin{bmatrix}
0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 \\
& & & &
& & & &
1 & 0 & \\
& & & &
0 & \\
& & & &
0 & & & &
\end{bmatrix},
b_{-2} = \begin{bmatrix}
0 & \\
0 & 1 & 0 \\
& 0 & \\
& 0 & \\
& 1 & \\
& & & &
\end{bmatrix}, ..., \]

...
There are $2(2^n-2)+1$ anti-diagonal operators $b_k$ ($k = 0, \pm 1, \pm 2, \ldots, \pm (2^n-2)$) in an $n$-qubit spin system except the two operators $|0\rangle\langle 0|$ and $|2^n-1\rangle\langle 2^n-1|$. The two operators are anti-diagonal operators and also diagonal operators. They are usually assigned to diagonal operators. All these anti-diagonal operators are symmetrical and Hermitian operators. For every anti-diagonal matrix $b_k$ all its non-zero elements that take one are located along an anti-diagonal line of the matrix. The matrix $b_0$ is the main anti-diagonal matrix where all its $2^n$ non-zero elements taking one are located along the main anti-diagonal line. The two end points (row, column) of the main anti-diagonal line are $(0, 2^n-1)$ and $(2^n-1, 0)$ in the matrix $b_0$, respectively. There are only $(2^n-k)$ nonzero elements in the matrix $b_k$ (or $b_{-k}$) $(2^n-2 \geq k \geq 0)$ along the anti-diagonal line of the matrix. Actually, there is a unit difference between numbers of matrix element in two nearest anti-diagonal lines in a matrix. Thus, nonzero-element number of the anti-diagonal matrix $b_{k+1}$ is one less than that of the matrix $b_k$, and since the matrix $b_0$ has $2^n$ nonzero elements the matrix $b_k$ has $(2^n-k)$ nonzero elements. The two end points of the anti-diagonal line for the matrix $b_k$ are $(0, 2^n-1-k)$ and $(2^n-1-k, 0)$, respectively, and for the matrix $b_{-k}$ are $(k, 2^n-1)$ and $(2^n-1-k, 0)$, respectively. Denote that $x$ is row coordinate and $y$ column coordinate. Then the main anti-diagonal line is given by $x = -y + 2^n - 1$, and the anti-diagonal lines of the matrices $b_k$ and $b_{-k}$ are given by $x = -y + 2^n - 1 - k$ and $x = -y + 2^n - 1 + k$, respectively. Note that an anti-diagonal operator $b_k$ is symmetric and it has $(2^n-k)$ nonzero (one) elements. If the index $k$ is odd then the matrix $b_k$ must contain a diagonal element taking one. This diagonal element exactly locates at the position $(2^n-1-(k+1)/2, 2^n-1-(k+1)/2)$ along same anti-diagonal line of the matrix $b_k$. However, there is not any diagonal element in the anti-diagonal matrix $b_k$ with an even index $k$.

The unitary operator $B_k(\theta) = \exp(-i\theta b_k)$ built up with any Hermitian anti-diagonal operator $b_k$ by exponential mapping may be decomposed into a
sequence of the basic unitary operations. This may be achieved by expressing the anti-diagonal operator as a sum of basic product operators. Several important unitary operators $B_k(\theta)$ are given below with their explicit decomposition. Note that an anti-diagonal operator $b_{\pm k}$ with $k \geq 2^{n-1}$ first can be simplified by

$$ (b_{\pm k})_{2^n \times 2^n} = \left( \frac{1}{2} E_1 \pm I_{1z} \right) \bigotimes (b_{\pm (k-2^{n-1})})_{2^{n-1} \times 2^{n-1}} $$

where $b_{\pm k} \equiv (b_{\pm k})_{2^n \times 2^n}$ with the subscript $2^n \times 2^n$ indicating dimensional size of the matrix $b_k$. Now the index $(k - 2^{n-1}) < 2^{n-1}$ and one needs to express only the $(n-1)$-qubit anti-diagonal operator $(b_{\pm (k-2^{n-1})})_{2^{n-1} \times 2^{n-1}}$ in the product operator form. Therefore, explicit product operator expressions will be given only for those operators $b_{\pm k}$ with $k < 2^{n-1}$ below.

(a) The main anti-diagonal operator $b_0$. The operator $b_0$ can be easily expressed as

$$ b_0 = 2^n I_{1x} \bigotimes I_{2x} \bigotimes \ldots \bigotimes I_{nx}. \quad (18) $$

This is a simple anti-diagonal operator often used in previous papers [2, 3, 5, 6]. With the help of the single-spin rotation operations and the recursive relation (10) the unitary operator $B_0(\theta) = \exp(-i\theta b_0)$ can be easily decomposed into an efficient sequence of one- and two-qubit gates.

(b) The operator $b_{\pm 1}$. The product operator expression for the operator $b_1$ is slightly complicated. There is a recursive relation for the anti-diagonal operator $b_1$:

$$ b_1 \equiv (b_1)_{2^n \times 2^n} = 2^{n-1} I_{1x} I_{2x} \ldots I_{n-1x} \bigotimes (\frac{1}{2} E_n + I_{nz}) $$

$$ + (b_1)_{2^{n-1} \times 2^{n-1}} \bigotimes (\frac{1}{2} E_n - I_{nz}). $$

Using this recursive relation one can express the operator $b_1$ as a sum of $n$ commutative product operators:

$$ b_1 = \left( \frac{1}{2} E_1 + I_{1z} \right) \bigotimes \left( \frac{1}{2} E_2 - I_{2z} \right) \bigotimes \ldots \bigotimes \left( \frac{1}{2} E_n - I_{nz} \right) $$

$$ + 2I_{1x} \bigotimes \left( \frac{1}{2} E_2 + I_{2z} \right) \bigotimes \left( \frac{1}{2} E_3 - I_{3z} \right) \bigotimes \ldots \bigotimes \left( \frac{1}{2} E_n - I_{nz} \right) $$

$$ + 2^2 I_{1x} I_{2x} \bigotimes \left( \frac{1}{2} E_3 + I_{3z} \right) \bigotimes \left( \frac{1}{2} E_4 - I_{4z} \right) \bigotimes \ldots \bigotimes \left( \frac{1}{2} E_n - I_{nz} \right) + \ldots $$

$$ + 2^{n-2} I_{1x} \bigotimes I_{2x} \bigotimes \ldots \bigotimes I_{n-2x} \bigotimes \left( \frac{1}{2} E_{n-1} + I_{n-1z} \right) \bigotimes \left( \frac{1}{2} E_n - I_{nz} \right) $$
\[ + 2^{n-1} I_{1x} \otimes I_{2x} \otimes \ldots \otimes I_{n-1x} \otimes \left( \frac{1}{2} E_n + I_{nz} \right). \]  

(19)

Since all these product operators in the operator \( b_1 \) are commutative the corresponding unitary operator \( B_1(\theta) \) is decomposed as a sequence of \( n \) basic unitary operations,

\[
B_1(\theta) = \exp[-i\theta(\frac{1}{2} E_1 + I_{1z}) \otimes (\frac{1}{2} E_2 - I_{2z}) \otimes \ldots \otimes (\frac{1}{2} E_n - I_{nz})] \\
\times \exp[-i\theta 2 I_{1x} \otimes (\frac{1}{2} E_2 + I_{2z}) \otimes (\frac{1}{2} E_3 - I_{3z}) \otimes \ldots \otimes \left( \frac{1}{2} E_n - I_{nz} \right)] \\
\times \exp[-i\theta 2^2 I_{1x} I_{2x} \otimes (\frac{1}{2} E_3 + I_{3z}) \otimes (\frac{1}{2} E_4 - I_{4z}) \otimes \ldots \otimes \left( \frac{1}{2} E_n - I_{nz} \right)] \times \ldots \\
\times \exp[-i\theta 2^{n-2} I_{1x} I_{2x} \ldots I_{n-2x} \otimes (\frac{1}{2} E_{n-1} + I_{n-1z}) \otimes (\frac{1}{2} E_n - I_{nz})] \\
\times \exp[-i\theta 2^{n-1} I_{1x} I_{2x} \ldots I_{n-1x} \otimes (\frac{1}{2} E_n + I_{nz})].
\]

(20)

In a similar way, the anti-diagonal operator \( b_{-1} \) also can be expressed as a sum of \( n \) commutative product operators,

\[
b_{-1} = \left( \frac{1}{2} E_1 - I_{1z} \right) \otimes \left( \frac{1}{2} E_2 + I_{2z} \right) \otimes \ldots \otimes \left( \frac{1}{2} E_n + I_{nz} \right) \\
+ 2 I_{1x} \otimes \left( \frac{1}{2} E_2 - I_{2z} \right) \otimes \left( \frac{1}{2} E_3 + I_{3z} \right) \otimes \ldots \otimes \left( \frac{1}{2} E_n + I_{nz} \right) \\
+ 2^2 I_{1x} I_{2x} \otimes \left( \frac{1}{2} E_3 - I_{3z} \right) \otimes \left( \frac{1}{2} E_4 + I_{4z} \right) \otimes \ldots \otimes \left( \frac{1}{2} E_n + I_{nz} \right) \ldots \\
+ 2^{n-2} I_{1x} \otimes I_{2x} \otimes \ldots I_{n-2x} \otimes \left( \frac{1}{2} E_{n-1} - I_{n-1z} \right) \otimes \left( \frac{1}{2} E_n + I_{nz} \right) \\
+ 2^{n-1} I_{1x} \otimes I_{2x} \otimes \ldots \otimes I_{n-1x} \otimes \left( \frac{1}{2} E_n - I_{nz} \right),
\]

and corresponding unitary operator \( B_{-1}(\theta) \) therefore is decomposed as a sequence of \( n \) basic unitary operations.

(c) The operator \( b_{zk} \) with \( k = 2^l \) (\( l = 1, 2, \ldots, n - 1 \)). First consider the operator \( b_k \) with an even index \( k \). The number of nonzero (one) elements of the matrix \( b_k \) along the anti-diagonal line is \( 2^n - k \). If the index \( k \) is even then so is \( 2^n - k \). If now the matrix \( b_k \) is blocked by a \( 2 \times 2 \) submatrix one can see this blocked matrix \( b_k \) is still an anti-diagonal blocked matrix, and the nonzero blocked submatrix is \( 2I_x = \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \) along the anti-diagonal line. Therefore, the matrix \( b_k \) may be written as \((b_k)_{2^n \times 2^n} = (b_{k'})_{2^{n-1} \times 2^{n-1}} \otimes 2I_{nz}\) with index \( k' = k/2 \), and \( b_{k'} \) is also an anti-diagonal matrix. If \( k' \) is still even then the matrix \( b_k \) can be further written.
as \((b_k)_{2^n \times 2^n} = (b_k')_{2^{n-2} \times 2^{n-2}} \bigotimes 2I_{n-1} \bigotimes 2I_{nx}\) with index \(k'' = k/4\). Generally, for the operator \(b_k\) with \(k = 2^l\) \((l = 1, 2, ..., n - 1)\) number of nonzero elements is \((2^n - 2^l)\) on the anti-diagonal line. Then the operator \(b_{2^l}\) can be reduced to the form

\[
b_{2^l} = (b_1)_{2^{n-l} \times 2^{n-l}} \bigotimes 2^l I_{n-l+1} I_{n-l+2} ... I_{nx}.
\]  

(21)

Particularly the matrix \(b_2\) can be written as \(b_2 = (b_1)_{2^{n-1} \times 2^{n-1}} \bigotimes 2I_{nx}\). Because the operator \((b_1)_{2^{n-1} \times 2^{n-1}}\) can be further expressed as a sum of \((n-l)\) commutative product operators, as shown in (b), the operator \(b_{2^l}\) now is written as a sum of \((n-l)\) commutatable product operators and hence the unitary operator \(B_k(\theta) = \exp(-i\theta b_k)\) with \(k = 2^l\) \((l = 1, 2, ..., n - 1)\) can be decomposed as a sequence of \((n-l)\) basic unitary operations. In a similar way, the anti-diagonal operator \(b_{-k}\) with \(k = 2^l\) can be reduced to the form

\[
b_{-2^l} = (b_{-1})_{2^{n-l} \times 2^{n-l}} \bigotimes 2^l I_{n-l+1} I_{n-l+2} ... I_{nx},
\]

where \((b_{-1})_{2^{n-l} \times 2^{n-l}}\) can be further expressed as a sum of \((n-l)\) commutative product operators. Therefore, the unitary operator \(B_{-k}(\theta) = \exp(-i\theta b_{-k})\) with \(k = 2^l\) can also be decomposed as a sequence of \((n-l)\) basic unitary operations.

Generally, an anti-diagonal operator \(b_k\) with an even index \(k = 2^{k_1-1} + \ldots + 2^{k_l-2} + ... + 2^{k_{1}}\) can be simplified by

\[
b_k = (b_k')_{2^{n-k_1} \times 2^{n-k_1}} \bigotimes 2^{k_1} I_{n-k_1+1} I_{n-k_1+2} ... I_{nx} \tag{22}
\]

with the odd index \(k' = 2^{k_{1}-1-k_1} + 2^{k_{l-2}-k_1} + ... + 2^{k_{2}-k_1} + 1\).

(d) A general operator \(b_k\). In (c) it is shown that an anti-diagonal operator \(b_k\) with an even index \(k\) can be reduced to another lower-dimensional anti-diagonal operator with an odd index. Here consider the operator \(b_k\) with an odd index \(k\). The operator \(b_k\) always can be written in the form

\[
(b_k)_{2^n \times 2^n} = \begin{cases} 
  (b_{k_1/2})_{2^{n-2} \times 2^{n-2}} \bigotimes 2I_{n-1} \bigotimes (\frac{1}{2}E_n + I_{nz}) \\
  + (b_1)_{2^{n-1} \times 2^{n-1}} \bigotimes (\frac{1}{2}E_n - I_{nz}), & \text{if } k_1 \text{ is even,} \\
  (b_{l_1/2})_{2^{n-2} \times 2^{n-2}} \bigotimes 2I_{n-1} \bigotimes (\frac{1}{2}E_n - I_{nz}) \\
  + (b_{l_1})_{2^{n-1} \times 2^{n-1}} \bigotimes (\frac{1}{2}E_n + I_{nz}), & \text{if } l_1 \text{ is even,}
\end{cases} \tag{23}
\]

where \(k_1 = (k - 1)/2\) and \(l_1 = (k + 1)/2\). The number of nonzero elements keep unchanged before and after the reduction: \((2^n - k) = (2^{(n-1)} - k_1) + \ldots + (2^{(n-1)} - l_1) + 1\).
The \( n \)-qubit anti-diagonal operator \((b_k)_{2^n \times 2^n}\) now consists of one term containing \((n - 1)\)-qubit anti-diagonal operator \((b_{k_1})_{2^{n-1} \times 2^{n-1}}\) (or \((b_{k_1})_{2^{n-1} \times 2^{n-1}}\)) and another term containing \((n - 2)\)-qubit anti-diagonal operator \((b_{k_1/2})_{2^{n-2} \times 2^{n-2}}\) (or \((b_{k_1/2})_{2^{n-2} \times 2^{n-2}}\)). Note that the two terms are commutable to each other. This is an advantage of the decomposition based on the recursive relation (23). Image that using (23) an \( n \)-qubit anti-diagonal operator at the first step is decomposed as a sum of two \((n - 1)\)-qubit anti-diagonal operator terms, then at the second step the two \((n - 1)\)-qubit anti-diagonal operators are decomposed as four \((n - 2)\)-qubit anti-diagonal operator terms, and so on, in the final the \( n \)-qubit operator \(b_k\) would be a sum of \(2^{n-1}\) commutable basic product operators if the decomposition could be carried out to the final \((n - 1)\)th step. However, the recursive relation (23) shows that although the \( n \)-qubit anti-diagonal operators can be further reduced to only one \((n - 2)\)-qubit anti-diagonal operator term instead of two terms. Then term number of the basic product operators in the completely decomposed operator \(b_k\) is not really more than \(2^{n-1}\). For some specific cases one may use conveniently the recursive relation (23) to decompose an anti-diagonal operator \(b_k\) as a sum of polynomially many basic product operators. Take the anti-diagonal operators \(b_{\pm k}\) with index \(k = 2^r \pm 2^m\) \((n > r > m = 0, 1, 2, ..., n - 1)\) as an example.

For the index \(k = 2^r \pm 2^m\) the operator \(b_k\) is first reduced to the form
\[
(b_k)_{2^n \times 2^n} = (b_{2^r-2^m})_{2^{n-m} \times 2^{n-m}} \bigotimes 2^m I_{n-m+1} I_{n-m+2} ... I_{n-r},
\]
as shown in (22). Then consider the anti-diagonal operator \((b_{2^r+1})_{2^r \times 2^r}\) with \(t = n - m\) and \(l = r - m\). It follows from (23) that there is a recursive relation for the operator \((b_{2^r+1})_{2^r \times 2^r}\):

\[
(b_{2^r+1})_{2^r \times 2^r} = (b_{2^r-1})_{2^{r-1} \times 2^{r-1}} \bigotimes (\frac{1}{2} E_t - I_t) + (b_1)_{2^{r-1} \times 2^{r-1}} \bigotimes 2^{r-1} I_{l-1} I_{l+1} I_{l+2} ... I_{l-1} \bigotimes (\frac{1}{2} E_t + I_t).
\]

This is because in (23) \(k_1 = (k - 1)/2 = 2^{r-1}\) and \((b_{2^r-1/2})_{2^{r-2} \times 2^{r-2}}\) can be further reduced to the operator \((b_1)_{2^{r-1} \times 2^{r-1}}\), as shown in (e). This relation directly leads to the product operator expression for the operator \((b_{2^r+1})_{2^r \times 2^r}\):

\[
(b_{2^r+1})_{2^r \times 2^r} = (b_{2^r-1})_{2^{r-1} \times 2^{r-1}} \bigotimes 2^{r-1} I_{l-1} I_{l+1} I_{l+2} ... I_{l-1} \bigotimes (\frac{1}{2} E_t + I_t) + (b_{2^{r-1}})_{2^{r-1} \times 2^{r-1}} \bigotimes 2^{r-2} I_{l-1} I_{l+1} I_{l+2} ... I_{l-1} \bigotimes (\frac{1}{2} E_t - I_t) \bigotimes (\frac{1}{2} E_t - I_t).
\]
The operator \((b_1)_{2^t-1 \times 2^t} \otimes 2^{t-3} I_{t-l+1} I_{t-l+2} \ldots I_{t-3} \otimes (\frac{1}{2} E_{t-2} + I_{t-2})\) 
\(\otimes (\frac{1}{2} E_{t-1} - I_{t-1}) \otimes (\frac{1}{2} E_{t} - I_{t}) + \ldots\) 
\(+ (b_1)_{2^t-1 \times 2^t} \otimes 2 I_{t-l+1} \otimes (\frac{1}{2} E_{t-l+2} + I_{t-l+3}) \otimes (\frac{1}{2} E_{t-l+3} - I_{t-l+3})\) 
\(\otimes \ldots \otimes (\frac{1}{2} E_{t} - I_{t})\) 
\(+ (b_1)_{2^t-1 \times 2^t} \otimes (\frac{1}{2} E_{t-l+1} + I_{t-l+1}) \otimes (\frac{1}{2} E_{t-l+2} - I_{t-l+2}) \otimes \ldots\) 
\(\otimes (\frac{1}{2} E_{t} - I_{t})\).

The operator \((b_{2^t+1})_{2^t \times 2^t}\) now is a sum of \((l + 1)\) commutative operators. Since the operator \((b_1)_{2^t-1 \times 2^t}\) can be expressed as a sum of \((t - l)\) commutative product operators, as shown in (b), and \((b_2)_{2^t-1 \times 2^t}\) as a sum of \((t - l - 1)\) commutative product operators, as shown in (c), then the operator \((b_{2^t+1})_{2^t \times 2^t}\) is a sum of \((l + 1)(t - l) - 1\) commutative product operators. Now taking \(t = n - m\) and \(l = r - m\) one sees the operator \((b_k)_{2^n \times 2^n}\) with \(k = 2^r + 2^m\) is a sum of \((r - m + 1)(n - r) - 1\) commutative product operators. Thus, the unitary operator \(B_k(\theta)\) can be decomposed as a sequence of \((r - m + 1)(n - r) - 1\) basic unitary operations. In an analogous way, it can be shown that the unitary operator \(B_{-k}(\theta)\) can be also decomposed as a sequence of \((r - m + 1)(n - r) - 1\) basic unitary operations.

From (23) there is also a recursive relation for the operator \((b_{2^t-1})_{2^t \times 2^t}\) :

\[(b_{2^t-1})_{2^t \times 2^t} = (b_{2^t-1-1})_{2^{t-1} \times 2^{t-1}} \otimes (\frac{1}{2} E_t + I_{t+2}) + (b_{2^{t-1}})_{2^{t-1} \times 2^{t-1}} \otimes (\frac{1}{2} E_{t} - I_{t+2}).\]

Then using this relation the product operator expression for the operator \((b_{2^t-1})_{2^t \times 2^t}\) is given by

\[(b_{2^t-1})_{2^t \times 2^t} = (b_{2^{t-2}})_{2^{t-2} \times 2^{t-2}} \otimes (\frac{1}{2} E_{t-1} - I_{t-1}) \otimes (\frac{1}{2} E_{t} + I_{t+2})\]

\(\otimes (\frac{1}{2} E_{t-l+3} + I_{t-l+3}) \otimes \ldots \otimes (\frac{1}{2} E_{t} + I_{t+2})\)

\(+ (b_1)_{2^t-l+1 \times 2^t-l+1} \otimes (\frac{1}{2} E_{t-l+2} + I_{t-l+3})\)

\(\otimes (\frac{1}{2} E_{t-l+3} + I_{t-l+3}) \otimes \ldots \otimes (\frac{1}{2} E_{t} + I_{t+2}).\)
Because the operator \((b_{2^l-m})_{2^t-m \times 2^t-m}\) \((m = 1, 2, ..., l - 1)\) can be expressed as a sum of \((t - l)\) commutative product operators the operator \((b_{2^t-1})_{2^t \times 2^t}\) is clearly a sum of \(l(t - l) + 1\) commutative product operators. Then the operator \(b_k\) with \(k = 2^r - 2^m\) is a sum of \((r - m)(n - r) + 1\) commutative product operators and hence its unitary operator \(B_k(\theta)\) can be decomposed as a sequence of \((r - m)(n - r) + 1\) basic unitary operations.

The above results suffice to construct an efficient subspace-selective multiple-quantum unitary operator (5) that transfers completely an unknown state from any subspace \(S_{2^q}(m)\) \((m \neq n/2)\) to the largest subspace \(S_{2^q}(n/2)\) of the Hilbert space of an \(n\)-qubit spin system.

A general anti-diagonal operator also can be decomposed using the recursive relation (23) in an analogue way. But by using only the recursive relation (23) it is usually not convenient to obtain an efficient decomposition for the unitary operator \(B_k(\theta) = \exp(-i\theta b_k)\) with a general anti-diagonal operator \(b_k\). It can be proved that a general anti-diagonal operator can be converted into another anti-diagonal operator with a different index by a proper unitary transformation, and for a general anti-diagonal operator \(b_k\) with an odd index \(k = 2^{k_{l-1}} + 2^{k_{l-2}} + ... + 2^{k_1} + 1\) \((n - 1 > k_{l-1} > k_{l-2} > ... > k_1 \geq 1)\) its unitary operator \(B_k(\theta) = \exp(-i\theta b_k)\) can be generally expressed as

\[
B_k(\theta) = U_k \exp(-i\theta \overline{b}_{k_1}) U_k^+ \tag{24}
\]

where the operator \(\overline{b}_{k_1}\) is a symmetric and Hermitian anti-diagonal operator similar to the anti-diagonal operator \(b_1\) and \(U_k\) is a unitary operator dependent on the index \(k\). The anti-diagonal line of the operator \(\overline{b}_{k_1}\) is the same as that of the operator \(b_1\), but number of nonzero elements taking one along the anti-diagonal line in the operator \(\overline{b}_{k_1}\) is only \((2^n - k)\) instead of \((2^n - 1)\) of the operator \(b_1\). The \((2^n - k)\) nonzero elements locate symmetrically at the center of the anti-diagonal line and each of two ends of the anti-diagonal line has \((k - 1)/2\) zero elements. Note that the index \(k\) is odd. Just like \(b_1\) the symmetric matrix \(\overline{b}_{k_1}\) has a diagonal element at position \((2^{n-1} - 1, 2^{n-1} - 1)\) and hence the operator \(\overline{b}_{k_1}\) also contains the diagonal operator \(D_{2^{n-1}-1}\). The diagonal operator \(D_{2^{n-1}-1}\) is commutable with both the operators \(b_1\) and \(\overline{b}_{k_1}\). The unitary operator \(\overline{D}_{k_1}(\theta) = \exp(-i\theta \overline{b}_{k_1})\) can be decomposed efficiently. Just like the subspace-selective multiple-quantum operator (27) (see next section) the Hermitian operator \(\overline{b}_{k_1}\) can be expressed as

\[
(\overline{b}_{k_1} - D_{2^{n-1}-1}) = [\overline{g}_k, (b_1 - D_{2^{n-1}-1})]_+ = \overline{g}_k(b_1 - D_{2^{n-1}-1}) + (b_1 - D_{2^{n-1}-1})\overline{g}_k
\]
where the diagonal operator $\mathcal{G}_k$ is given by

$$\mathcal{G}_k = \text{Diag}(0, ..., 0_{(k-1)/2-1}; 1_{(k-1)/2}, ..., 1_{(2^{n-1}-1) - 1}; 0_{(2^{n-1}-1), ..., 0_{N-1}}).$$

As shown in section 3.1, the unitary diagonal operator $\mathcal{G}_k(\theta) = \exp(-i\theta\mathcal{G}_k)$ can be decomposed efficiently into a sequence of the $l-$qubit selective rotation operations $C_{l,t,m}(\theta)$ ($l = 1, 2, ..., n$) with number less than $2n$. Since both the two operators $(\mathcal{b}_{k_1} - D_{2^{n-1} - 1})$ and $(\mathcal{b}_1 - D_{2^{n-1} - 1})$ do not contain any diagonal operator components and both the two operators $G_k(b_1 - D_{2^{n-1} - 1})$ and $(b_1 - D_{2^{n-1} - 1})\mathcal{G}_k$ have not any overlapping nonzero matrix element it follows from the unitary transformation (38) and the decomposition formula (41) in next section that the unitary operator $\mathcal{B}_{k_1}(\theta) = \exp(-i\theta\mathcal{b}_{k_1})$ can be efficiently decomposed as

$$\mathcal{B}_{k_1}(\theta) = C_{2^{n-1} - 1}(\theta) \exp[-i\theta(\mathcal{b}_{k_1} - D_{2^{n-1} - 1})]$$

$$= C_{2^{n-1} - 1}(\theta) \exp[-i\frac{1}{2}\theta(b_1 - D_{2^{n-1} - 1})/L]\mathcal{G}_k(\pi)$$

$$\times \exp[i\frac{1}{2}\theta(b_1 - D_{2^{n-1} - 1})/L]\mathcal{G}_k(\pi)^{-1} + O(L^{-1})$$

$$= C_{2^{n-1} - 1}(\theta) \exp[-i\frac{1}{2}\theta b_1/L]\mathcal{G}_k(\pi)$$

$$\times \exp(i\frac{1}{2}\theta b_1/L)\mathcal{G}_k(\pi)^{-1} + O(L^{-1}).$$

(25)

For a modest number $L = \varepsilon^{-1}$ this expansion of the unitary operator $\mathcal{B}_{k_1}(\theta)$ can fast converge. As shown in (b), the unitary operator $\exp(-i\frac{1}{2}\theta b_1/L)$ is a sequence of $n$ basic unitary operations. Then the unitary operator $\mathcal{B}_{k_1}(\theta)$ can be decomposed as a sequence of the basic unitary operations with number less than $6\varepsilon^{-1}n$.

It can be proved that the unitary operator $U_k$ in (24) with the index $k = 2^{k_1-1} + 2^{k_2-2} + ... + 2^{k_1} + 1$ ($n = 1 > k_{l-1} > k_{l-2} > ... > k_1 \geq 1$ and $1 < l \leq n - 1$) can be written as

$$U_k = \begin{cases} 
\exp(i\frac{\pi}{2}b_{j_1}) \exp(i\frac{\pi}{2}b_{j_2}) \exp(i\frac{\pi}{2}b_{j_3}) 
\times \cdots \times \exp(i\frac{\pi}{2}b_{j_{l-2}}), \text{ if } l - 1 \text{ is even,} \\
\exp(i\frac{\pi}{2}b_{j_1}) \exp(i\frac{\pi}{2}b_{j_2}) \exp(i\frac{\pi}{2}b_{j_3}) 
\times \cdots \times \exp(i\frac{\pi}{2}b_{j_{l-1}}) \exp(i\frac{\pi}{2}b_0), \text{ if } l - 1 \text{ is odd,}
\end{cases}$$

(26)

where the indices $j_1 = 2^{k_{l-1}-1}, j_2 = 2^{k_{l-2}-1}, ..., j_{l-1} = 2^{k_1-1}$. Since the unitary operator $\exp(-i\theta b_{j_l})$ with $j = 2^l$ ($l = 1, 2, ..., n - 1$) can be decomposed as a
sequence of \((n - l)\) basic unitary operations, as shown in (c), then the unitary operator \(\exp(i\pi/2b_{\pm jm})\) with index \(j_m = 2^{k-m-1}\) in (26) can be decomposed into a sequence of \((n - k_{l-m} + 1)\) basic unitary operations. Therefore, number of the basic unitary operations in the unitary operator \(U_k\) (26) is \((n - k_{l-1} + 1) + (n - k_{l-2} + 1) + ... + (n - k_1 + 1)\) if \(l - 1\) is even or \((n - k_{l-1} + 1) + (n - k_{l-2} + 1) + ... + (n - k_1 + 1) + 1\) if \(l - 1\) is odd. Note that \((n - k_{l-1} + 1) + (n - k_{l-2} + 1) + ... + (n - k_1 + 1) + 1 < (l - 1)n + 1 < n^2\). The unitary operator \(U_k\) (26) then can be decomposed into a sequence of the basic unitary operations with number less than \(n^2\).

Therefore, the expansion (25) of the unitary operator \(\exp(-i\theta b_{k1})\) and the decomposition (26) of the unitary operator \(U_k\) show that the unitary operator \(B_k(\theta)\) (24) built up with a general anti-diagonal operator \(b_k\) can be expressed as a sequence of the basic unitary operations with number less than \(2n^2 + 6\epsilon^{-1}n\), and quantum-circuit complexity for the unitary operator is \(O(2n^2 + 6\epsilon^{-1}n)\).

3.3 The subspace-selective multiple-quantum operators

The Hermitian multiple-quantum operator \(Q_{pm}\) in the subspace-selective multiple-quantum unitary operator \(U_{pm}(\theta) = \exp(-i\theta Q_{pm})\) (5) can be generated by the anti-commutator of the diagonal and anti-diagonal operators:

\[
Q_{pm} = \sum_{l=0}^{d(m)-1} Q_{pml} = \frac{1}{2}[b_k, g_m] + = \frac{1}{2}(g_mb_k + b_k g_m),
\]

(27)

where the anti-diagonal operator \(b_k\) needs to be chosen properly and the diagonal operator \(g_m \in S_{zq}(m) \times S_{zq}(m)\) so that the \(p\)-quantum unitary operator \(U_{pm}(\theta)\) built up with the Hermitian \(p\)-quantum operator \(Q_{pm}\) is selectively applied on both the state subspace \(S_{zq}(m)\) and another larger subspace \(S_{zq}(m+p)\). It needs first to show how to choose the anti-diagonal operator \(b_k\) to generate the Hamiltonian operator \(Q_{pm}\). Here consider only the case \(0 \leq m < n/2\). For the case \(n \geq m > n/2\) the multiple-quantum operator \(Q_{pm}\) can be constructed with the operator \(b_{-k}\) in place of the operator \(b_k\) and the final result is similar. For convenience the anti-diagonal operator \(b_k \equiv (b_k)_{N \times N}\) (\(N = 2^n\)) is written as

\[
b_k \equiv Adiag(1_{[0,N-k-1]}, 1_{[1,N-k-2]}, ..., 1_{[N-k-1,0]}; 0_{[N-k,N-1]}, ..., 0_{[N-1,N-k]}).
\]

Suppose that the operator \(b_k\) is chosen properly so that the operator \(g_mb_k\) is
given by

\[
g_m b_k = \text{Diag}(0, \ldots, 0_{l_m - 1}; 1_{l_m}, \ldots, 1_{L_m}; 0_{L_m + 1}, \ldots, 0_{N-1}) \\
\times \text{Adiag}(1_{[0, N-k-1]}, 1_{[1, N-k-2]}, \ldots, 1_{[N-k-1, 0]}; \\
0_{[N-k, N-1]}, \ldots, 0_{[N-1, N-k]})
\]

\[
= \text{Adiag}(0_{[0, N-k-1]}; \ldots, 0_{[l_m-1, N-k-1-l_m+1]}; \\
1_{[l_m, N-k-1-l_m]}; \ldots, 1_{[L_m, N-k-1-L_m]}; \\
0_{[L_m+1, N-k-1-L_m-1]}, \ldots, 0_{[N-k-1, 0]}; 0_{[N-k, N-1]}, \ldots, 0_{[N-1, N-k]})
\]

and the operator is written as

\[
b_k g_m = \text{Adiag}(1_{[0, N-k-1]}, 1_{[1, N-k-2]}, \ldots, 1_{[N-k-1, 0]}; 0_{[N-k, N-1]}, \ldots, 0_{[N-1, N-k]}) \\
\times \text{Diag}(0, \ldots, 0_{l_m - 1}; 1_{l_m}, \ldots, 1_{L_m}; 0_{L_m + 1}, \ldots, 0_{N-1})
\]

\[
= \text{Adiag}(0_{[0, N-k-1]}; \ldots, 0_{[l_m-1, N-k-1-l_m+1]}; \\
1_{[N-k-1-l_m, L_m]}; \ldots, 1_{[N-k-1-l_m, L_m]}; \\
0_{[N-k-1-l_m+1, l_m-1]}, \ldots, 0_{[N-k-1, 0]}; 0_{[N-k, N-1]}, \ldots, 0_{[N-1, N-k]})
\]

Obviously, the index \(N - 1 - k\) must be greater than the index \(L_m\). Both the operators \(g_m b_k\) and \(b_k g_m\) are also anti-diagonal operators. Their nonzero elements taking one are also along the same anti-diagonal line of the matrix \(b_k\). Each of the two operators has only \(d(m)\) nonzero matrix elements, which number is exactly dimensional size of the state subspace \(S_{2q}(m)\). The operator \((g_m b_k + b_k g_m)\) is clearly a symmetric and Hermitian operator and can be written as

\[
(g_m b_k + b_k g_m)
\]

\[
= \text{Adiag}(0_{[0, N-k-1]}; \ldots, 0_{[l_m-1, N-k-1-l_m+1]}; \\
1_{[l_m, N-k-1-l_m]}; 0_{[l_m+1, N-k-1-l_m+1]}; \ldots, 0_{[N-k-1-l_m-1, l_m+1]}; \\
1_{[N-k-1-l_m, l_m]}; 0_{[N-k-1-l_m+1, l_m-1]}; \ldots, 0_{[N-k-1, 0]}; \\
0_{[N-k, N-1]}, \ldots, 0_{[N-1, N-k]})
\]

\[
+ \text{Adiag}(0_{[0, N-k-1]}; \ldots, 0_{[l_m, N-k-1-l_m]}; \\
1_{[l_m+1, N-k-1-l_m-1]}; 0_{[l_m+2, N-k-1-l_m-2]}; \ldots, 0_{[N-k-1-l_m-2, l_m+2]}; \\
1_{[N-k-1-l_m-1, l_m+1]}; 0_{[N-k-1-l_m, l_m]}; \ldots, 0_{[N-k-1, 0]}; \\
0_{[N-k, N-1]}, \ldots, 0_{[N-1, N-k]}) + \ldots
\]

\[
+ \text{Adiag}(0_{[0, N-k-1]}; \ldots, 0_{[L_m-1, N-k-1-L_m+1]};
\]

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Therefore, the operator \((g_m b_k + b_k g_m)\) can be expressed as a sum of \(d(m)\) commutative and symmetric anti-diagonal operators at most, each of which has only two elements taking one along the same anti-diagonal line of the matrix \(b_k\). Such an anti-diagonal operator can be written in terms of the usual computational basis \(\{|\varphi_k\rangle\} : \\
\text{Adiag}(0|\varphi_0\rangle, \ldots, 0|\varphi_{d(m)-1}\rangle) = |\varphi_{l_m+l'}\rangle\langle\varphi_{N-k-1-l_m-l'}| + |\varphi_{N-k-1-l_m-l'}\rangle\langle\varphi_{l_m+l'}|,
\) where the index \(l' = 0, 1, \ldots, L_m - l_m\) \((L_m - l_m = d(m) - 1)\) and the base \(|\varphi_{l_m+l'}\rangle\) belongs to the state subspace \(S_{2q}(m)\). If both the operators \(g_m b_k\) and \(b_k g_m\) have common nonzero matrix elements then the operator \((g_m b_k + b_k g_m)\) is a sum of commutative and Hermitian anti-diagonal operators with number less than \(d(m)\). If the basis state \(|\varphi_{N-k-1-l_m-l'}\rangle\) belongs to another subspace \(S(M_m + p)\) this anti-diagonal operator is a state-selective \(p\)–quantum operator that applies only on both the two basis states \(|\varphi_{l_m+l'}\rangle\) and \(|\varphi_{N-k-1-l_m-l'}\rangle\). Now it is required that both the operators \(g_m b_k\) and \(b_k g_m\) have not any common nonzero matrix elements so that the operator \((g_m b_k + b_k g_m)\) is a sum of the commutative anti-diagonal operators with number \(d(m)\) exactly. Then the index \(N - 1 - k > 2L_m\), and the operator \((g_m b_k + b_k g_m)\) can be written in terms of the usual computational basis \(\frac{1}{2}(g_m b_k + b_k g_m) = \sum_{l'=0}^{d(m)-1} \frac{1}{2}(|\varphi_{l_m+l'}\rangle\langle\varphi_{N-k-1-l_m-l'}| + |\varphi_{N-k-1-l_m-l'}\rangle\langle\varphi_{l_m+l'}|).
\) Note that all the \(d(m)\) basis states \(|\varphi_{l_m+l'}\rangle\) \((l' = 0, 1, \ldots, d(m) - 1)\) in (28) belong to the subspace \(S_{2q}(m)\). If now all the \(d(m)\) basis states \(|\varphi_{N-k-1-l_m-l'}\rangle\) in (28) belong to the subspace \(S_{2q}(m + p)\) whose dimensional size is larger.
than that of $S_{2q}(m)$, the operator $\frac{1}{2}(g_mb_k + b_kg_m)$ is a subspace-selective multiple-quantum operator which applies only to both the two subspaces $S_{2q}(m)$ and $S_{2q}(m + p)$. This can be seen more clearly by comparing the operator (28) with the operator (27) and the multiple-quantum operators (3) and (5). Therefore, the condition that the operator $\frac{1}{2}(g_mb_k + b_kg_m)$ is the subspace-selective $p$-quantum operator $Q_{pm}$ (5) selectively applied to both the subspaces $S_{2q}(m)$ and $S_{2q}(m + p)$ is that in addition to $N - 1 - k > 2L_m$ the index $k$ for the anti-diagonal operator $b_k$ must satisfy

$$l_{m+p} \leq N - k - 1 - l_m - l' \leq L_{m+p}, \; l' = 0, 1, ..., d(m) - 1. \quad (29)$$

Note that $L_m = l_m + d(m) - 1$ and $L_m < l_{m+p}$ for $0 \leq m + p \leq n/2$ and $p \geq 1$. The condition $N - 1 - k > 2L_m$ always holds if the condition $L_m < l_{m+p} \leq N - k - 1 - l_m - (d(m) - 1)$ holds. Thus, the condition (29) is a general condition to determine the proper index $k$ for the anti-diagonal operator $b_k$ that is used to construct the subspace-selective $p$-quantum operator $Q_{pm}$ (27).

Consider the $n$-qubit spin system with an even qubit number $n$. Then the largest subspace for the system is $S_{2q}(n/2)$. Let $S_{2q}(m + p) = S_{2q}(n/2)$. Then the condition (29) is rewritten as

$$l_{n/2} \leq N - k - 1 - l_m - l' \leq L_{n/2}, \; l' = 0, 1, ..., d(m) - 1. \quad (30)$$

The condition (30) shows that $l_{n/2} \leq N - k - 1 - l_m \leq L_{n/2}$ if $l' = 0$ and if $l' = d(m) - 1$ then $l_{n/2} \leq N - k - 1 - L_m \leq L_{n/2}$, and since $N - k - 1 - l_m > N - k - 1 - (l_m + 1) > ... > N - k - 1 - L_m$ one has for $l' = 0, 1, ..., d(m) - 1$,

$$l_{n/2} \leq N - k - 1 - L_m < ... < N - 1 - k - l_m \leq L_{n/2}.$$ 

Therefore, the lower bound $(k_m)_{\text{min}}$ and upper bound $(k_m)_{\text{max}}$ for the index $k \equiv k_m$ of the subspace $S_{2q}(m)$ for $m = 0, 1, ..., n/2 - 1$ are given by

$$(k_m)_{\text{min}} = N - l_m - L_{n/2} - 1 \quad \text{and} \quad (k_m)_{\text{max}} = N - L_m - l_{n/2} - 1,$$

and hence the index $k_m$ is bounded on by

$$N - l_m - l_{n/2} - d(n/2) \leq k_m \leq N - l_m - l_{n/2} - d(m). \quad (31)$$

The condition (31) shows that range of the index $k_m$ is equal to $\Delta k_m = (k_m)_{\text{max}} - (k_m)_{\text{min}} = d(n/2) - d(m)$. For a different state subspace $S_{2q}(m)$
the distance $\Delta k_m$ is different, and the maximum and minimum $\Delta k_m$ are $\Delta k_0 = d(n/2) - d(0) = \left(\frac{n}{n/2}\right) - 1$ and $\Delta k_{n/2-1} = d(n/2) - d(n/2-1) = \frac{2}{n/2} \left(\frac{n}{n/2}\right)$, respectively, and moreover $\Delta k_0 > \Delta k_1 > ... > \Delta k_{n/2-1}$. Note that $2l_{n/2} + d(n/2) = \sum_{m=0}^{n} d(m) = \sum_{m=0}^{n} \left(\frac{n}{m}\right) = 2^n = N$. The condition (31) is reduced to the form

$$l_{n/2} - l_m \leq k_m \leq l_{n/2} - l_m + d(n/2) - d(m)$$

where $l_m = d(0) + d(1) + ... + d(m - 1)$ and $l_0 = 0$, and $l_{n/2} > l_{n/2-1} > ... > l_1 > l_0$. Now using the condition (32) one can determine the index $k_m$ for the desired operator $b_{k_m}$.

Suppose that the index $k_m = 2^{n-1}$. Since $N/2 = l_{n/2} + d(n/2)/2 > l_{n/2}$ the first inequality in the condition (32) always holds: $k_m = N/2 > l_{n/2} - l_m$. The second inequality is reduced to the form

$$d(n/2)/2 - l_m - d(m) \geq 0.$$

Therefore, the operator $b_{k_m}$ with $k_m = 2^{n-1}$ can be used to construct those $p$-quantum operators $Q_{pm}$ with index $m = 0, 1, ..., m_0$ where the maximum index $m_0$ is determined from the inequality (33):

$$l_{m_0+1} = \sum_{l=0}^{m_0} d(l) \leq \frac{1}{2} d(n/2).$$

As shown in section 3.2, the anti-diagonal operator $b_{k_m}$ with index $k_m = 2^{n-1}$ can be explicitly expressed as

$$b_{k_m} = (\frac{1}{2} E_1 + I_{1z}) \bigotimes 2^{n-1} I_{2x}I_{3x}...I_{nx}$$

and the corresponding unitary operator $B_{k_m}(\theta)$ therefore is a basic unitary operation,

$$B_{k_m}(\theta) = \exp[-i\theta (\frac{1}{2} E_1 + I_{1z}) \bigotimes 2^{n-1} I_{2x}I_{3x}...I_{nx}].$$

This quantum unitary operator is used to build up a subspace-selective $p$-quantum unitary operator $U_{pm}(\theta)$ (5) that can transfer any unknown state
that is in one of the subspaces \( S_{zq}(0), S_{zq}(1), \ldots, S_{zq}(m_0) \) into the largest subspace \( S_{zq}(n/2) \).

Next consider the situation \( m_0 < m \leq n/2 - 1 \). Since \( l_{n/2} - l_m = d(m) + d(m+1) + \ldots + d(n/2 - 1) \) the condition (32) is rewritten as

\[
d(m) + d(m+1) + \ldots + d(n/2 - 1) \leq k_m \leq d(m+1) + d(m+2) + \ldots + d(n/2). \tag{35}
\]

In particular, for \( m = n/2 - 1 \) the condition (35) is written as

\[
\left( \frac{n}{n/2 - 1} \right) \leq k_{n/2 - 1} \leq \left( \frac{n}{n/2} \right). \tag{36}
\]

By the minimum distance \( \Delta k_{n/2 - 1} = \frac{2}{n+2} \left( \frac{n}{n/2} \right) \) one may obtain the index \( k_m \) that satisfies (35) for each subspace \( S_{zq}(m) \) with \( m_0 < m \leq n/2 - 1 \). The minimum distance \( \Delta k_{n/2 - 1} \) is approximated by using the Starling’s formula

\[
n! \approx \sqrt{2\pi n} (n/e)^n \quad \text{for a large } n,
\]

and

\[
\log_2 \Delta k_{n/2 - 1} \approx n - \log_2 \left( \frac{1}{2} n \sqrt{n} \sqrt{\frac{\pi}{2}} \left( 1 + \frac{2}{n} \right) \right).
\]

Denote \( n_0 = \lfloor \log_2 \left( \frac{1}{2} n \sqrt{n} \sqrt{\frac{\pi}{2}} \left( 1 + \frac{2}{n} \right) \right) \rfloor \) as integer part of \( \log_2 \left( \frac{1}{2} n \sqrt{n} \sqrt{\frac{\pi}{2}} \left( 1 + \frac{2}{n} \right) \right) \). Then \( 2^{n-n_0 - 1} \leq \Delta k_{n/2 - 1} \leq 2^{n-n_0} \) and \( 2^{n_0} \sim n^{3/2} \). The minimum index \( (k_{n/2 - 1})_{\min} \) that satisfies (36) is approximated by the Starling formula

\[
(k_{n/2 - 1})_{\min} = \left( \frac{n}{n/2 - 1} \right) \approx \sqrt{2 \pi n} \frac{n}{n+2} \frac{1}{2} 2^n
\]

and

\[
\log_2 \left( \frac{n}{n/2 - 1} \right) \approx n - \log_2 \left( \sqrt{n} \sqrt{\frac{\pi}{2}} \left( 1 + \frac{2}{n} \right) \right).
\]

Let \( k_0 = \lfloor \log_2 \left( \sqrt{n} \sqrt{\frac{\pi}{2}} \frac{1}{2+2/n} \right) \rfloor \). Then \( 2^{n-k_0 - 1} \leq (k_{n/2 - 1})_{\min} \leq 2^{n-k_0} \) and \( 2^{k_0} \sim n^{1/2} \). Although taking \( k_{n/2 - 1} = 2^{n-k_0} \) the first inequality in (36) can be satisfied, the second inequality in (36) could not be satisfied. Now suppose that the index \( k_{n/2 - 1} = 2^{n-k_0} + \mu 2^{n-n_0 - 1}, \mu \) is an integer to be determined. Then there is an integer \( \mu \) such that the index \( k_{n/2 - 1} \) satisfies the
condition (36). There is always an integer \( \mu_0 \) such that \( 2^{n-k_0-1} + \mu_0 2^{n-n_0-1} < (k_{n/2-1})_{\min} \leq 2^{n-k_0-1} + (\mu_0 + 1) 2^{n-n_0-1} \). The integer \( \mu_0 \) equals \( [(k_{n/2-1})_{\min} - 2^{n-k_0-1})/2^{n-n_0-1}] \). Because \( 2^{n-k_0-1} + \mu_0 2^{n-n_0-1} \leq (k_{n/2-1})_{\min} \) and \( 2^{n-n_0-1} \leq \Delta k_{n/2-1} \) there must be \( 2^{n-k_0-1} + (\mu_0 + 1) 2^{n-n_0-1} \leq (k_{n/2-1})_{\min} + \Delta k_{n/2-1} = d(n/2) \). By taking \( \mu = \mu_0 + 1 \) the index \( k_{n/2-1} = 2^{n-k_0-1} + \mu 2^{n-n_0-1} \) satisfies the condition (36). Generally, suppose that there is an integer \( \mu_0 \) such that \( 2^{n-k_0-1} + \mu_0 2^{n-n_0-1} < d(m) + d(m + 1) + ... + d(n/2 - 1) \leq 2^{n-k_0-1} + (\mu_0 + 1) 2^{n-n_0-1} \). Because \( 2^{n-n_0-1} \leq \Delta k_{n/2-1} \) \( \leq \Delta k_m \) there holds \( 2^{n-k_0-1} + (\mu_0 + 1) 2^{n-n_0-1} < d(m) + d(m + 1) + ... + d(n/2 - 1) + \Delta k_m = d(m + 1) + d(m + 1) + ... + d(n/2) \). Therefore, the index \( k_m = 2^{n-k_0-1} + \mu_m 2^{n-n_0-1} \) with \( \mu_m = \mu_0 + 1 \) satisfies the condition (35). For \( m_0 < m \leq n/2 - 1 \) the upper bound for the index \( k_m \) is obtained from the condition (35) by taking \( m = m_0 + 1 \):

\[
\begin{align*}
  k_m & \leq d(m_0 + 2) + d(m_0 + 3) + ... + d(n/2) \\
  & = l_{n/2} + d(n/2) - d(0) - d(1) - ... - d(m_0) - d(m_0 + 1) \\
  & < N/2.
\end{align*}
\]

This is because \( \sum_{l=0}^{m_0+1} d(l) > \frac{1}{2} d(n/2) \) and \( \sum_{l=0}^{m_0} d(l) \leq \frac{1}{2} d(n/2) \), as shown in (33). Since \( k_m < 2^{n-1} \) the index \( k_m \) can be expanded as a binary number:

\[
\begin{align*}
  k_m &= 2^{n-k_0-1} + \mu_m 2^{n-n_0-1} \\
  &= a_{n-2} 2^{n-2} + a_{n-3} 2^{n-3} + ... + a_{n-n_0-1} 2^{n-n_0-1}
\end{align*}
\]

(37)

where \( a_l = 0, 1 \) \( (l = n-n_0-1, n-n_0, ..., n-2) \). The anti-diagonal operator \( b_{km} \) with the index (37) then can be expressed as, as can be seen in (22),

\[
(b_{km})_{2^n \times 2^n} = (b_{km}^\prime)_{2^{n_0+1} \times 2^{n_0+1}} \bigotimes 2^{n-n_0-1} I_{n_0+2x} I_{n_0+3x} ... I_{n_x}
\]

where \( \mu_m = a_{n-2} 2^{n_0-1} + a_{n-3} 2^{n_0-2} + ... + a_{n-n_0-1} 2^{0} \) and the anti-diagonal operator \( b_{km}^\prime \) has a dimensional size \( 2^{n_0+1} \times 2^{n_0+1} \). Because \( 2^{n_0} \sim n^{3/2} \) the operator \( (b_{km}^\prime)_{2^{n_0+1} \times 2^{n_0+1}} \) can be expressed as a sum of \( \sim n^{3/2} \) commutative product operators at most using the recursive relation (23) in section 3.2. Therefore, the operator \( b_{km} \) is also a sum of \( \sim n^{3/2} \) commutative product operators at most.

Furthermore, if using the general decomposition (24) for a general anti-diagonal operator the unitary operator \( \exp(-i \theta b_{km}) \) with the index \( k_m \) (37)
can be decomposed into a sequence of the basic unitary operations with a complexity only $O(2(n_0 + 1)^2 + 6\varepsilon^{-1}(n_0 + 1))$, which is $\sim O(\log^2 n)$.

For an $n$-qubit spin system with an odd qubit number the largest subspaces are $S_{zq}(n/2 - 1/2)$ and $S_{zq}(n/2 + 1/2)$. Any state in one of the two largest subspaces can be converted unitarily into another largest subspace by a unitary transformation with $n$ single-spin unitary operations: $U = \prod_{k=1}^n \exp(-i\pi I_{k_x})$. This unitary transformation is also available for the complete quantum-state transfer between any pair of symmetric subspaces $S_{zq}(m)$ and $S_{zq}(n - m)$ in a general $n$-qubit spin system. Thus, it needs only to consider those subspaces $S_{zq}(k_m)$ with $0 \leq k_m \leq (n - 1)/2$. Take $S_{zq}(m + p) = S_{zq}(n/2 - 1/2)$. Now the minimum distance $\Delta k_{(n-1)/2-1} = d(n/2 - 1/2) - d((n-1)/2 - 1) = \frac{4}{n+3} \left( \frac{n}{n-1} \right)$ and is approximated by

$$\log_2 \Delta k_{(n-1)/2-1} \approx n - \log_2 \left\{ \sqrt{\frac{\pi n + 3 (1+n)\sqrt{n-1}}{4}} \right\} \times \sqrt{\frac{(1 + \frac{1}{n})^n}{\sqrt{[1 + \frac{1}{n-1}]^{n-1}}}}.$$

Now let $n_0 = \lfloor \log_2 \sqrt{\frac{\pi n + 3 (1+n)\sqrt{n-1}}{4}} \rfloor \sqrt{(1 + \frac{1}{n})^n / \sqrt{[1 + \frac{1}{n-1}]^{n-1}}}$. Note that $(1 + \frac{1}{n})^n \approx e$ for a large integer $n$. Then $2^{n_0} \sim n^{3/2}$. Therefore, for the case that the qubit number $n$ is odd the operator $b_{k_m}$ with $k_m = 2^{n_0} - 1$ is still used to construct those $p$-quantum operators $Q_{pm}$ (27) with index $m = 0, 1, \ldots, m_0$, but now the maximum index $m_0$ is determined from the inequality: $\sum_{l=0}^{m_0} d(l) \leq \frac{1}{4} d((n-1)/2)$, and when $m_0 < m < n/2 - 1/2$ the index $k_m$ is still given by (37). The complexity of quantum circuit of the unitary operator $\exp(-i\theta b_{k_m})$ is also $\sim O(\log^2 n)$.

For a general subspace $S_{zq}(m + p)$ instead of the largest subspace in an $n$-qubit spin system the index $k$ of the operator $b_k$ used to construct the $p$-quantum operator $Q_{pm}$ (27) is generally determined from the general condition (29), and the unitary operator $\exp(-i\theta b_k)$ is decomposed as a sequence of the basic unitary operations by the general decomposition (24), and the complexity of quantum circuit of the unitary operator $\exp(-i\theta b_k)$ is $O(2n^2 + 6n\varepsilon^{-1})$.

Once the unitary operator $\exp(-i\theta b_{k_m})$ with the anti-diagonal operator $b_{k_m}$ is expressed as an efficient sequence of the basic unitary operations the
subspace-selective $p-$quantum unitary operator $U_{ppn}(\theta)$ (5) can be easily decomposed as an efficient sequence of the basic unitary operations. A general unitary transformation with a sequence of selective rotation operations \( \{C_k(\theta_k)\} \) can help simplify the decomposition. The unitary transformation has been given in Ref.[6]:

\[
U_o(\theta_0, \theta_1, ..., \theta_{m-1})\rho_I(t)U_o(\theta_0, \theta_1, ..., \theta_{m-1})^{-1} = \rho_I(t) - \sum_{k=0}^{m-1} (1 - \cos \theta_k)D_k + i\sum_{k=0}^{m-1} D_k \sin \theta_k + \sum_{k=0}^{m-1m-1} \sum_{l=0}^{m-1} [(1 - \cos \theta_k)(1 - \cos \theta_l) + \sin \theta_k \sin \theta_l]D_k \rho_I(t)D_l + \sum_{l>k=0}^{m-1} i[\sin \theta_k(1 - \cos \theta_l) - \sin \theta_l(1 - \cos \theta_k)](D_k \rho_I(t)D_l - D_l \rho_I(t)D_k) \tag{38}
\]

where the diagonal unitary operation $U_o(\theta_0, \theta_1, ..., \theta_{m-1}) = \prod_{k=0}^{m'-1} C_k(\theta_k)$. Now setting $U_o(\theta_0, \theta_1, ..., \theta_{m'-1}) = G_m(\pi)$ and $\rho_I(t) = b_k$ and inserting them into the unitary transformation (38) one obtains

\[
G_m(\pi)b_kG_m(\pi)^{-1} = b_k - 2[b_k, g_m]_+ + 4 \sum_{k'} \sum_{l'} D_{k'}b_kD_{l'}, \tag{39}
\]

where $D_{k'}, D_{l'} \in S_{zq}(m) \times S_{zq}(m)$. Since an anti-diagonal operator $b_k$ with an even index $k$, e.g., $k_m$ does not contain any diagonal operator component, that is, all the diagonal elements of the matrix $b_k$ are equal to zero, there must be $D_{k'}b_kD_{k'} = (b_k)_{k'k}D_{k'} = 0$ for any diagonal operator $D_{k'}$. On the other hand, there also holds: $D_{k'}b_{km}D_{l'} = 0 \ (k' \neq l')$, $D_{k'}, D_{l'} \in S_{zq}(m) \times S_{zq}(m)$ (0 ≤ $m < n/2$). The matrix element of $D_{k'}b_kD_{l'}$ is given by

\[
(D_{k'}b_kD_{l'})_{ij} = \sum_l \sum_s \delta_{ik'}\delta_{ik'}(b_k)_{ls}\delta_{l'i'}\delta_{j'i'} = \delta_{ik'}(b_k)_{k'i'}\delta_{j'i'}.
\]

The element is not zero only when $i = k'$ and $j = l'$ and the indices $k'$ and $l'$ satisfy the anti-diagonal line equation of the matrix $b_k$ : $k' = -l' + N - 1 - k$. 

34
Since $D_k, D_l \in S_z^q(m) \times S_z^q(m)$ the indices $k'$ and $l'$ satisfy $l_m \leq k', l' \leq L_m$ and $k' + l' \leq 2L_m$. However, it follows from the anti-diagonal line equation that $k' + l' = N - 1 - k > 2L_m$ because the condition (29) shows that the index $N - 1 - k > 2L_m$. Therefore, the operator $D_k b_{k_m} D_l$ is zero for those anti-diagonal operators $b_{k_m}$ used to build up the $p-$quantum operator $Q_{pm}$. Then the unitary transformation (39) can be further reduced to the form

$$G_m(\pi)b_{k_m}G_m(\pi)^{-1} = b_{k_m} - 2[b_{k_m}, g_m].$$ (40)

With the help of the unitary transformation (40) and the Trotter-Suzuki formula [13, 14] the subspace-selective $p-$quantum unitary operator $U_{pm}(\theta) = \exp(-i\theta Q_{pm})$ can be decomposed as

$$U_{pm}(\theta) = \exp(-i\frac{1}{2}[g_m, b_{k_m}]_+)$$

$$= \exp[-i\frac{1}{4}\theta(b_{k_m} - G_m(\pi)b_{k_m}G_m(\pi)^{-1})]$$

$$= [\exp(-i\frac{1}{4}\theta b_{k_m}/L)G_m(\pi)$$

$$\times \exp(i\frac{1}{4}\theta b_{k_m}/L)G_m(\pi)^{-1}]^L + O(L^{-1}).$$ (41)

Note that norm for the operators $b_{k_m}$ and $g_m$ and their commutator $[b_{k_m}, g_m]$ equals one, that is, $\|b_{k_m}\| = 1$, $\|g_m\| = 1$, and $\|[b_{k_m}, g_m]\| = 1$. Then for a modest number $L = \varepsilon^{-1}$ the expansion (41) for the $p-$quantum unitary operator $U_{pm}(\theta)$ can converge quickly. The computational complexity for the quantum circuit of the $p-$quantum unitary operator $U_{pm}(\theta)$ is therefore dependent on that of the unitary operations $B_{k_m}(\theta)$ and $G_m(\theta)$. It is shown in section 3.1 that the unitary operation $G_m(\theta)$ can be decomposed into a sequence of $2n$ basic unitary operations at most. For the situation that an unknown state in a subspace is transferred into the largest subspace of the Hilbert space of the $n-$qubit spin system the complexity of quantum circuit of the unitary operator $B_{k_m}(\theta)$ is $\sim O(\log^2 n)$, and for a general case that an unknown state is transferred from a subspace into a larger subspace the complexity is $O(2n^2 + 6n\varepsilon^{-1})$. Therefore, it follows from (41) that the subspace-selective $p-$quantum unitary operator $U_{pm}(\theta)$ can be expressed as a sequence of the basic unitary operations with complexity $O(2(2n^2 + 6n\varepsilon^{-1})\varepsilon^{-1} + 4n\varepsilon^{-1})$.

4. Discussion
It has been shown that any unknown quantum state can be efficiently transferred from a state subspace into a larger state subspace of the Hilbert space of an $n$–qubit spin system by a subspace-selective multiple-quantum unitary transformation, but the Grover quantum search algorithm [4, 15, 16] shows indirectly that the inverse process usually is hard one. This multiple-quantum transition process is similar to evolution process from nonequilibrium state to equilibrium state in a closed quantum system, although the former is a unitary process and the latter a non-unitary and irreversible process [17]. This result might be helpful for understanding nonequilibrium processes such as protein folding process in nature where energy effect usually is not dominating from the point view of quantum dynamics. By the efficient subspace-selective multiple-quantum unitary transformation that can transfer efficiently any state from a small subspace into the largest subspace of the Hilbert space the search space of the quantum search problem can be reduced from the whole Hilbert space to its largest subspace. With the help of the results in the paper and the auxiliary oracle unitary operation it can be shown that the quantum search algorithm [2, 6] based on quantum dynamics is at least as powerful as those quantum search algorithms including the Grover quantum search algorithm [4, 16] and adiabatic quantum search algorithm [18] in a pure quantum-state system because the former algorithm needs only to find which subspace the marked state is in among the $(n + 1)$ subspaces of the Hilbert space. The diagonal and the anti-diagonal unitary operators will have an extensive application in constructing efficient quantum circuits for permutation operations of a symmetry group and the unitary operations of a cyclic group.

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