Introduction to the multiple-quantum operator spaces

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The multiple-quantum NMR spectroscopy has an extensive application in determination of the bio-macro-molecular structures and in the investigation of the properties of a variety of physical materials. In quantum computation the multiple-quantum transition processes have been used to construct the quantum circuits, quantum algorithms, and quantum simulations. The multiple-quantum operator algebra spaces are closely related to the symmetries of a multiple-spin quantum system. They may have an important effect on the multiple-quantum transition processes and the multiple-quantum NMR spectroscopy of the spin system. Here gives a brief introduction to the multiple-quantum operator algebra spaces.

1. The multiple-quantum operator algebra spaces

Symmetry in quantum mechanics is important. Symmetry of the Hilbert state space of a quantum system is one of the most important factors to help the unitary quantum dynamics to speed up a quantum computation [1, 2]. Symmetry leads to that the whole Hilbert space of a quantum system or equivalently the whole Liouville operator space of a quantum ensemble is decomposed into many small subspaces. This further simplifies the unitary quantum dynamics of the quantum system. Thus, people may use some symmetric properties of a quantum system to simplify investigation of the unitary time evolution process of the system. For example, the rotating symmetry in the spin internal space results in that the total spin angular momentum of a spin system is constant [3, 4]. Symmetry is closely related to degeneracy of energy eigenvalues in a quantum system. In an uncoupled or weakly coupled multiple-spin system (there is not any orbital angular momentum) it is usually related to degeneracy of eigenvalues of the total spin angular momentum as the total spin angular momentum commutes with the spin Hamiltonian of the system. There is also another important symmetry, i.e., the interchange symmetry between a pair of spins in an uncoupled multiple-spin system [3, 4, 5]. This interchange symmetry leads to that eigenvalues of the total spin angular momentum and its z-component are degenerate in an uncoupled multiple-spin system. The multiple-quantum operator algebra spaces [6] that will be briefly introduced below are closely related to the interchange symmetry in a multiple-spin system.

According to quantum mechanics [3] a quantum system may be described by a wave function. There is a Hilbert state space for the quantum system and each quantum state to describe the quantum system belongs to the Hilbert space. A dynamical variable then is represented by a linear operator in quantum mechanics. On the other hand, a quantum system which may be a pure-state
system or a quantum ensemble also may be described by a density operator. This density-operator-based description has been used extensively in the NMR spectroscopy [7] and a number of other research fields, whose research object usually is a quantum ensemble. In quantum mechanics both the descriptions based on a wave function and on a density operator are compatible with the fundamental and universal principle that both a closed quantum system and its ensemble obey the same unitary quantum dynamics [1, 2, 6, 9, 11]. A spin system usually has a finite-dimensional Hilbert space. To describe generally the time evolution process of a quantum system with a finite-dimensional Hilbert space it could be more convenient to use a complete set of the base operators to expand the density operator of the system [8]. Such a complete set of the base operators form an operator space called the Liouville operator space [7]. This Liouville operator space (sometime it is called the Hilbert operator space) corresponds to the Hilbert state space of the same quantum system. Obviously, any dynamical variable such as the Hamiltonian of the quantum system also may be expanded in terms of the base operators. Therefore, the symmetric structure and property of the Liouville operator space may be helpful for simplifying investigation of the time evolution process of a quantum system. For a multiple-spin system both the rotating symmetry in the spin internal space and the interchange symmetry could be exploited to help the investigation. Due to the two symmetries and especially the interchange symmetry of a multiple-spin system the Liouville operator space of an \( n \)-spin system may be generally divided into several operator subspaces [6]:

(i) The longitudinal magnetization and spin order (\( LOMSO \)) operator subspace

(ii) The zero-quantum operator subspace

(iii) The even-order multiple-quantum operator subspace

Here the largest subspace is the even-order multiple-quantum operator subspace which contains the first two subspaces. The second largest one is the zero-quantum operator subspace which contains the whole \( LOMSO \) operator subspace. The \( LOMSO \) operator subspace is the minimum subspace among the above three subspaces. This is a commutable subspace. It usually consists of all the diagonal operators of the Liouville operator space of a quantum system.

The usual observation in the multiple-quantum NMR spectroscopy is not correct that all zero-quantum coherence operators of a spin system form a closed operator subspace or that all zero-quantum coherence operators plus the longitudinal magnetization operators of a spin system form a closed operator subspace. A closed zero-quantum operator subspace must contain the whole \( LOMSO \) operator subspace, that is, it consists of all the zero-quantum coherence operators, longitudinal magnetization operators, longitudinal spin order operators, and the unity operator. Here the unity operator is a necessary component to form a closed operator algebra space.

Furthermore, each one of these three operator subspaces could be further divided into several smaller operator subspaces. In particular, the above zero-quantum operator subspace may be further divided into the \((n+1)\) selective zero-quantum operator subspaces for an \( n \)-spin \((I = 1/2)\) system [9], each one
of which is much smaller than the total zero-quantum operator subspace.

The conventional zero- and double-quantum operator subspaces [7] in a two-spin \((I = 1/2)\) system are very special. They are deduced based on the corresponding relations between them and the operator space of a single spin \((I=1/2)\) system. It is known that the operator space of a single-spin \((I=1/2)\) system is given by \(\{I_x, I_y, I_z\}\). It can turn out that for the operator commutation relations there exist the corresponding relations:

\[
\frac{1}{2}(I_{1z} - I_{2z}) \leftrightarrow I_z; \quad (I_{1x}I_{2x} + I_{1y}I_{2y}) \leftrightarrow I_y; \quad (I_{1x}I_{2y} - I_{1y}I_{2x}) \leftrightarrow I_x.
\]

It can be deduced from these corresponding relations that these three operators \(\{(I_{1x}I_{2y} - I_{1y}I_{2x}), (I_{1x}I_{2x} + I_{1y}I_{2y}), \frac{1}{2}(I_{1z} - I_{2z})\}\) form an operator space. This operator space is just the conventional zero-quantum operator space of a two-spin \((I = 1/2)\) system. Thus, the usual zero-quantum operator subspace of a two-spin system and the operator space of a single-spin system are isomorphic to each other. While one may use these corresponding relations to deduce the above zero-quantum subspace of a two-spin system, the subspace is very special. These corresponding relations can not be used to further deduce a general zero-quantum operator subspace in a complex spin system. Similarly, the conventional double-quantum operator subspace in a two-spin system is also very special. The corresponding relations similar to the above can not be used to further deduce a general even-order multiple-quantum operator subspace in a complex spin system.

The multiple-quantum operator spaces may be used to simplify the quantum simulation of a general spin quantum system. Consider the spin Hamiltonian of an \(n\)-qubit spin system. The spin Hamiltonian could not be in any one of the above three operator subspaces, but it is still in the Liouville operator space (here without considering the normalization condition), that is, the spin Hamiltonian still can be expanded in terms of the complete base operator set of the Liouville operator space. The unitary propagator of the spin Hamiltonian can be decomposed into a sequence of many elementary propagators. Obviously, complexity of the decomposition may be measured by the number of elementary propagators in the decomposed sequence. Then the multiple-quantum operator spaces may be used to decrease the number of elementary propagators in the decomposed sequence [6]:

(i) At first the unitary propagator (or the spin Hamiltonian) is converted into an element of the even-order multiple-quantum operator subspace by a unitary transformation.

(ii) The ever-order multiple-quantum unitary propagator then is converted into an element of the zero-quantum operator subspace by the ever-order multiple-quantum unitary transformation.

(iii) The zero-quantum unitary propagator finally is converted into an element of the \(LOMSO\) operator subspace by a zero-quantum unitary transformation.

One of the important properties of an operator algebra space is the closure property. This closure property leads directly to the fact that in a zero-quantum
operator subspace the product of any two zero-quantum operators is still a zero-quantum operator. This further leads to the fact that a unitary exponential operator generated by a hermite zero-quantum coherence operator is also a zero-quantum operator. Suppose that $Z_q$ is a hermite zero-quantum coherence operator. Then the unitary operator generated by the zero-quantum operator $Z_q$ is written as

$$U_{zq}(t) = \exp\{-iZ_q t\}.$$  \hfill (1)

Then it can turn out that this unitary operator $U_{zq}(t)$ is also a zero-quantum operator and is called the zero-quantum unitary operator. Denote $\{Z_a\}$ as the base operator set of the zero-quantum operator subspace. With the help of the closure property of a zero-quantum operator subspace one can prove that the following zero-quantum unitary transformation may be expanded in the zero-quantum operator subspace:

$$U_{zq}(t)Q_{zq}U_{zq}(t)^{-1} = \sum_a A_a Z_a,$$  \hfill (2)

where $Q_{zq}$ is a traceless and hermite zero-quantum operator, while the zero-quantum base operators $\{Z_a\}$ include the longitudinal magnetization operators $\{I_{kz}\}$ and spin order operators $\{2I_{kz}I_{lz}, 4I_{kz}I_{lz}I_{mz}, \ldots\}$ as well as the zero-quantum coherence operators $\{(ZQC)_k\}$. Then the unitary transformation may be explicitly written as

$$U_{zq}(t)Q_{zq}U_{zq}(t)^{-1} = \sum_{k=1}^n \Omega_k(t) I_{kz} + \sum_{k > l} J_{kl}(t) 2I_{kz}I_{lz}$$

$$+ \sum_{k > l > m} J_{klm}(t) 4I_{kz}I_{lz}I_{mz} + \ldots + J_{12...n}(t) 2^{n-1} I_{1z}I_{2z}...I_{nz} + \sum_k \beta_k(t)(ZQC)_k,$$  \hfill (3)

where $\Omega_k(t)$, $J_{kl}(t)$, $J_{klm}(t)$, $J_{12...n}(t)$, $\beta_k(t)$, etc., are the amplitude parameters. This formula shows that if the zero-quantum operator $Q_{zq}$ is a longitudinal magnetization operator, e.g., $I_{kz}$, then it can be converted into not only the longitudinal magnetization operators $\{I_{lz}\}$ but also many spin-order operators such as $2I_{kz}I_{lz}$, $4I_{kz}I_{lz}I_{mz}$, etc., as well as the zero-quantum coherence operators $\{(ZQC)_k\}$. This formula could be useful to analyze in theory some NMR experiments. Consider a conventional nuclear spin diffusion experiment in the NMR spectroscopy [7]. Here assume that the spin diffusion is driven by a zero-quantum Hamiltonian and the initial density operator of the spin diffusion process is taken as the longitudinal magnetization such as $I_{kz}$. Then during the spin diffusion process the initial longitudinal magnetization $I_{kz}$ is converted into other longitudinal magnetizations $\{I_{lz}\}$ with $l \neq k$. This is the desired result for the spin diffusion experiment. However, the formula (3) shows that the initial longitudinal magnetization also may be converted into the longitudinal spin orders and the zero-quantum coherences. These terms are undesired for the spin diffusion experiment and need to be cancelled in experiment. Therefore, during
the NMR detection of the spin diffusion one usually needs to use a purging pulse (or the homonuclear decoupling techniques) to cancel these undesired terms.

Note that the total zero-quantum subspace may be further divided into the \((n + 1)\) selective zero-quantum subspaces for an \(n\)-spin \((I=1/2)\) system. Then the above zero-quantum unitary transformation even can be greatly simplified. Denote \(S(k) \times S(k)\) as the \(k\)-th selective zero-quantum operator subspace for \(k = 0, 1, ..., n\) \([9]\). Now the hermite zero-quantum operator \(Z_q\) in Eq. (1) may be projected onto these \((n + 1)\) zero-quantum subspaces,

\[
Z_q = \sum_{k=0}^{n} Z_q(k).
\]

Since each one of these \((n + 1)\) zero-quantum operators \(\{Z_q(k)\}\) belongs to a different zero-quantum subspace, all these \((n + 1)\) zero-quantum operators commute with each other. Moreover, the \(k\)-th zero-quantum operator \(Z_q(k)\) can affect only those operators of the \(k\)-th zero-quantum subspace \(S(k) \times S(k)\). These results show that if the zero-quantum operator \(Q_{zq}^k\) belongs to the \(k\)-th zero-quantum subspace \(S(k) \times S(k)\), then the unitary transformation \(U_{zq}(t)Q_{zq}^kU_{zq}(t)^{-1}\) also generates a zero-quantum operator of the same subspace \(S(k) \times S(k)\) and it may be expanded as

\[
U_{zq}(t)Q_{zq}^kU_{zq}(t)^{-1} = \sum_a A_q^k Z_a(k),
\]

where \(\{Z_a(k)\}\) are the base operator set of the zero-quantum subspace \(S(k) \times S(k)\). Note that \(Z_q\) can be an arbitrary hermite zero-quantum operator. The formula (5) shows that the zero-quantum operator \(Q_{zq}^k\) evolves independently in its own selective zero-quantum subspace \(S(k) \times S(k)\) under the unitary transformation and any two selective zero-quantum subspaces do not mix with other each during the unitary transformation. This point is particularly important to analyze or design some NMR experiments such as the spin diffusion experiment. In general, the initial density operator of the spin diffusion process may not be in some selective zero-quantum subspace. But it can be projected onto these selective zero-quantum subspaces. Then one may use the formula (5) to calculate independently the time evolution process of the spin diffusion in each one of these selective zero-quantum subspaces. Therefore, the formula (5) may simplify the theoretical calculation of the time evolution process of the nuclear spin diffusion.

It is known that each one of these \((n + 1)\) selective zero-quantum subspaces \(\{S(k) \times S(k)\}\) for \(k = 0, 1, ..., n\) has a different dimensional size \(d(k)^2\) with the number \(d(k)\) given by \([10, 9]\)

\[
d(k) = \frac{n!}{k!(n-k)!}.
\]

For \(k \sim n/2\) these zero-quantum subspaces \(\{S(k) \times S(k)\}\) have exponentially large dimensions. If the spin diffusion occurs in these exponentially large zero-quantum subspaces, then thing becomes much complicated in the theoretical
treatment. On the other hand, it becomes much simpler to calculate the time evolution process of the spin diffusion if the spin diffusion is confined in the polynomially small zero-quantum subspaces or occurs mainly in these polynomially small subspaces. From the point of view of the NMR techniques it could not be difficult to prepare a spin system in some polynomially small zero-quantum subspaces in the spin diffusion experiment. The problem is how to measure efficiently the NMR signals from different zero-quantum subspaces.

The above theoretical strategy is not new that one uses the small zero-quantum subspaces to realize the NMR parameter measurement (or to calculate the corresponding time evolution process) in the nuclear spin diffusion experiment. In methodology it is really equivalent to the one that one uses small state subspaces of the Hilbert space to realize a quantum computation (or to calculate the corresponding time evolution process) in a pure-state quantum system. This strategy has been used to help to solve efficiently the quantum search problem [1, 2, 9] in quantum computation. Since the strategy may work in a pure-state quantum system and also in a quantum ensemble, the fundamental and universal quantum-mechanical principle that both a closed quantum system and its quantum ensemble obey the same unitary quantum dynamics [1, 2, 6, 9, 11] is of crucial importance when the strategy is used in quantum computation. This strategy might also be used to realize other quantum algorithms based on the unitary quantum dynamics and the quantum simulations. Here it will not be discussed in detail.

2. Some important properties of a zero-quantum coherence operator

A zero-quantum coherence operator also has some important properties which are independent of the multiple-quantum operator algebra spaces mentioned above. One of these important properties is stated as follows: any \( p \)-order quantum coherence operator does not change its quantum coherence order when it is acted on by a zero-quantum coherence operator. This property was first described qualitatively in the multiple-quantum NMR spectroscopy [12, 7]. Later, unknowing this description, the present author proved rigorously this property in a general spin system on the basis of the operator algebra theory [13]. With the help of the property of a zero-quantum coherence operator one can realize that the product operator formalism [14] can be used to analyze exactly the time evolution process in a strongly coupled spin system just like in a weakly coupled spin system [13]. The property also could be useful in quantum computation. However, it is necessary to have a strict mathematical proof for this property in a general spin system before the property can be used generally in the research fields such as the quantum simulation in quantum computation. Thus, only when these works [12, 7, 13] relevant to the property are put together, can the description for the property be considered to be complete.

Another important property of a zero-quantum coherence operator is that eigenvalues of any zero-quantum coherence operator are zero for both the ground state and the highest excited state in an \( n \)-spin \((I = 1/2)\) system.
3. The permutation transformation between the two different encodings for the product bases

The conventional computational basis set of an \( n \)-qubit spin system has been used extensively in quantum computation. This basis set is really the conventional product basis set of the \( n \)-spin \((I = 1/2)\) system that has been used extensively in the NMR spectroscopy \([10, 13]\). Obviously, each product base is an eigenstate of the total longitudinal magnetization operator \( I_z = \sum_{k=1}^{n} I_{kz} \) of the \( n \)-spin \((I=1/2)\) system. However, almost every eigenvalue of the longitudinal magnetization operator \( I_z \) is degenerate in the spin system. The longitudinal magnetization operator has a diagonal representation matrix in these product bases. Now these product bases are arranged suitably such that the diagonal matrix element, which is really an eigenvalue of the operator \( I_z \), descends (or does not increase) from top to bottom. Such an encoding for the product bases is more convenient to study the multiple-quantum transition processes \([9]\). It is different from the encoding of the conventional computational bases. Obviously, there is a permutation transformation between the two encodings of the product bases. It can turn out that this permutation transformation may be realized efficiently by the unitary operations generated by the anti-diagonal hermite matrices \([9]\).

Note added

It is generally hard to calculate exactly the time evolution process of the nuclear spin diffusion in solid in the NMR spectroscopy. The NMR Researchers tend to use a variety of approximation methods to treat in theory the nuclear spin diffusion, as can be seen in several works reported in the recent NMR meetings. The multiple-quantum operator spaces could provide a general theoretical frame to treat and explain the nuclear spin diffusion.

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