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The quantum state tomography on an NMR system

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Abstract

The quantum state tomography on an NMR system is analyzed. The evolution of a given system by its Hamiltonian during the measurement can be understood as the inverse evolution of physical observables. In this way the NMR signal is expressed as a composition of the ensemble averages of observables, which facilitates the build-up of the procedure for estimating the density operator. The widely used procedure in which only single-qubit rotations are used to get information about the ensemble averages of a quorum of observables is devoted and the lower bound for the number of experiments is obtained.

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1. Introduction

A density operator ρ contains all the physically significant information on a quantum system. If a density operator is given, we can calculate the ensemble average $\langle O \rangle$ of any arbitrary operator O on the Hilbert space of the system. Conversely, the density operator of the system can be estimated from ensemble averages of a set of observables which is called a *quorum* of observables [1]. This method of reconstructing the density operator is called *quantum state tomography*. The quantum state tomography has been developed with the advance of the quantum optics [2] and applied to other quantum systems, especially those expected to be quantum computers since the full descrip-

tion of the states of quantum bits is required to verify and increase the accuracy of quantum operations on a quantum computer.

In the field of the NMR quantum information processor [3,4], which leads the physical realization of a quantum computer up to present, the state tomography has been used from the primary stage [5]. Although the method has been used in many experiments (see Refs. [6–10]), there was no adequate analysis on the process [11,12].

In this Letter, the quantum state tomography on an NMR system is analyzed from a point of view that the Hamiltonian of a given system evolves the physical observables backward during the measurement. Unitary operations on the system can be considered as transforming the physical observables, too. In this context, the NMR signal is expressed as a composition of the ensemble averages of observables and the

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procedure for estimating the density operator is examined under the condition that only the combinations of the single-spin rotations are used to change a set of observables. The lower bound for the number of experiments necessary to constructing the density operator is obtained in this case.

2. State tomography on an NMR system

In NMR, the measured signal $S(t)$, by Fourier transforming which the NMR spectrum is obtained, is the time-varying current induced in a pick-up coil by the rotating bulk magnetization as

$$S(t) \propto \text{tr} \left[e^{-i\mathcal{H}t} \rho e^{i\mathcal{H}t} \sum_k (I_{kx} + i I_{ky}) \right], \quad (1)$$

where \mathcal{H} and ρ are the Hamiltonian of a spin system and the density operator at the beginning of the measurement respectively, and $I_{kx,y} = \frac{1}{2} \sigma_{kx,y}$ are the angular momentum operator of spin k , where σ represents the Pauli spin operators. Since the components $\sigma_{kx,y}$ of $e^{-i\mathcal{H}t} \rho e^{i\mathcal{H}t}$ are measured, it is not obvious what components of ρ are measured. The situation is the same when a unitary operator U are applied to get information about the ensemble averages of observables which cannot be estimated naturally.

To circumvent the difficulties, we used the identity

$$\begin{aligned} & \text{tr} \left[e^{-i\mathcal{H}t} \rho e^{i\mathcal{H}t} \sum_k (I_{kx} + i I_{ky}) \right] \\ &= \text{tr} \left[\rho e^{i\mathcal{H}t} \sum_k (I_{kx} + i I_{ky}) e^{-i\mathcal{H}t} \right]. \end{aligned}$$

This may be interpreted as the measured operators are not $\sum_k (I_{kx} + i I_{ky})$ but $e^{i\mathcal{H}t} \sum_k (I_{kx} + i I_{ky}) e^{-i\mathcal{H}t}$, which can be calculated more easily than $e^{-i\mathcal{H}t} \rho e^{i\mathcal{H}t}$ when the Hamiltonian \mathcal{H} is specified. Likewise, the effect of U on ρ can be translated to that on observables. Since it is obvious that which operators are measured and smaller number of terms are involved in calculation, this approach is advantageous to establish and analyze the state tomography on the NMR system.

The NMR Hamiltonian is usually composed of the Zeeman term by external field and the spin–spin interactions, which are expressed naturally in terms of the spin angular momentum operators, that is, the Pauli

spin operators. Therefore, it is logical to take products of a set of the identity and Pauli spin operators, $\{\mathbf{1}, \sigma_x, \sigma_y, \sigma_z\}$, as a quorum of observables. Now, we calculate Eq. (1) explicitly for the Hamiltonians of one-, two-, and three-spin systems on the assumption that spins are weakly coupled, and present the formulae of the density operator reconstruction for one- and two-spin systems using the combinations of $\pi/2$ rotations of a single spin about the axes x and y as a set of unitary transforms.

3. Example: one-spin system

The Hamiltonian \mathcal{H}_1 of a one-spin system consists of a single Zeeman term, which can be written as

$$\mathcal{H}_1 = \frac{1}{2} \omega \sigma_z, \quad (2)$$

where ω is the resonance frequency of the nuclear spin in the external magnetic field. Since

$$\exp\left(\pm i \frac{\omega}{2} \sigma_z t\right) = \mathbf{1} \cos \frac{\omega t}{2} \pm \sigma_z \sin \frac{\omega t}{2},$$

the NMR signal is

$$S^1(t) \propto \{\text{tr}[\rho \sigma_x] + i \text{tr}[\rho \sigma_y]\} e^{i\omega t}, \quad (3)$$

which is oscillating at the frequency ω and $\langle \sigma_x \rangle$ and $\langle \sigma_y \rangle$ are obtained in practice by Fourier transforming $S^1(t)$ and integrating the real and imaginary spectra, respectively. To reconstruct the density operator, we need to know $\langle \mathbf{1} \rangle$ and $\langle \sigma_z \rangle$ which are not directly measurable in NMR among a quorum of observables for a single spin, $\{\mathbf{1}, \sigma_x, \sigma_y, \sigma_z\}$. The ensemble average $\langle \mathbf{1} \rangle$ is determined by $\text{tr}[\rho] = 1$ and $\langle \sigma_z \rangle$ can be measured through the rotations of ρ by $X = \exp(-i \frac{\pi}{2} \sigma_x)$ or $Y = \exp(-i \frac{\pi}{2} \sigma_y)$. As mentioned above, these unitary transforms convert the observables σ_x and σ_y into σ_z and the signal becomes

$$S^X(t) \propto \{\text{tr}[\rho \sigma_x] - i \text{tr}[\rho \sigma_z]\} e^{i\omega t} \quad (4)$$

by X and

$$S^Y(t) \propto \{\text{tr}[\rho \sigma_z] + i \text{tr}[\rho \sigma_y]\} e^{i\omega t} \quad (5)$$

by Y . From S^1 , S^X , and S^Y , the ensemble averages of operators σ_x , σ_y , and σ_z can be obtained

$$\langle \sigma_x \rangle = c \text{avg}(\text{Re}[S^1(0)], \text{Re}[S^X(0)]), \quad (6a)$$

$$\langle \sigma_y \rangle = c \text{avg}(\text{Im}[S^1(0)], \text{Im}[S^Y(0)]), \quad (6b)$$

$$\langle \sigma_z \rangle = c \text{avg}(-\text{Im}[S^1(0)], \text{Re}[S^Y(0)]), \quad (6c)$$

where $\text{avg}(a, b)$ means an average of a and b . The factor c depends on experimental details such as a receiver gain, the amount of spins and so on, but can be set to a moderate number since the identity operator is not observed and the comparison of quantities such as a fidelity does not require the absolute value. After determining the factor c , the density operator of a single spin can be estimated by

$$\rho = \frac{1}{2} \mathbf{1} + \langle \sigma_x \rangle \sigma_x + \langle \sigma_y \rangle \sigma_y + \langle \sigma_z \rangle \sigma_z. \quad (7)$$

4. Example: two-spin system

The Hamiltonian of a weakly interacting two-spin system is

$$\mathcal{H}_2 = \frac{\omega_1}{2} \sigma_{1z} + \frac{\omega_2}{2} \sigma_{2z} + \frac{\pi}{2} J_{12} \sigma_{1z} \sigma_{2z}, \quad (8)$$

where J_{12} is a scalar coupling constant. Since all three terms in the Hamiltonian commute each other, we can easily calculate Eq. (1) to get

$$\begin{aligned} S^{11}(t) \propto & \{ [\text{tr}(\rho \sigma_{1x}) + \text{tr}(\rho \sigma_{1x} \sigma_{2z})] \\ & + i [\text{tr}(\rho \sigma_{1y}) + \text{tr}(\rho \sigma_{1y} \sigma_{2z})] \} e^{i(\omega_1 + \pi J_{12})t} \\ & + \{ [\text{tr}(\rho \sigma_{1x}) - \text{tr}(\rho \sigma_{1x} \sigma_{2z})] \\ & + i [\text{tr}(\rho \sigma_{1y}) - \text{tr}(\rho \sigma_{1y} \sigma_{2z})] \} e^{i(\omega_1 - \pi J_{12})t} \\ & + \{ [\text{tr}(\rho \sigma_{2x}) + \text{tr}(\rho \sigma_{1z} \sigma_{2x})] \\ & + i [\text{tr}(\rho \sigma_{2y}) + \text{tr}(\rho \sigma_{1z} \sigma_{2y})] \} e^{i(\omega_2 + \pi J_{12})t} \\ & + \{ [\text{tr}(\rho \sigma_{2x}) - \text{tr}(\rho \sigma_{1z} \sigma_{2x})] \\ & + i [\text{tr}(\rho \sigma_{2y}) - \text{tr}(\rho \sigma_{1z} \sigma_{2y})] \} e^{i(\omega_2 - \pi J_{12})t}, \end{aligned} \quad (9)$$

where $\sigma_{1x} \equiv \sigma_{1x} \otimes \mathbf{1}_2$, $\sigma_{2x} \equiv \mathbf{1}_1 \otimes \sigma_{2x}$, etc., and $\mathbf{1}_1$ and $\mathbf{1}_2$ mean identity operators for the first and second spins, respectively. Notice that the coupling term $\pi J_{12} \sigma_{1z} \sigma_{2z}$ splits the spectral lines and makes $\sigma_{1x} \sigma_{2z}$, $\sigma_{1y} \sigma_{2z}$, $\sigma_{1z} \sigma_{2x}$, and $\sigma_{1z} \sigma_{2y}$ observable.

Since the quorum of observables for two-spin system is

$$\{\mathbf{1}, \sigma_x, \sigma_y, \sigma_z\} \otimes \{\mathbf{1}, \sigma_x, \sigma_y, \sigma_z\},$$

it is necessary to measure the ensemble averages of sixteen observables for constructing the density

operator and this can be done by a set of unitary transform on ρ as a single-spin case. If we take as a set of unitary transform the standard nine experiments where the unitary transforms are **11**, **X1**, **Y1**, **1X**, **1Y**, **XX**, **XY**, **YX**, and **YY** where the first and second letters indicate the unitary transform applying to the first and second spin respectively, the ensemble averages of all fifteen observables except the identity operator can be obtained from the measured quantities using Table 1, where the abbreviations come from the expression of the NMR signal after a unitary transform U ,

$$\begin{aligned} S^U(t) \propto & (S_{1r}^U + i S_{1i}^U) e^{i(\omega_1 + \pi J_{12})t} \\ & + (S_{2r}^U + i S_{2i}^U) e^{i(\omega_1 - \pi J_{12})t} \\ & + (S_{3r}^U + i S_{3i}^U) e^{i(\omega_2 + \pi J_{12})t} \\ & + (S_{4r}^U + i S_{4i}^U) e^{i(\omega_2 - \pi J_{12})t}. \end{aligned} \quad (10)$$

Since each observable is measured several times through the standard nine experiments, it can be expected that some subset of experiments are enough to estimate ρ . Actually four experiments among the standard set, for example **X1**, **Y1**, **1X**, and **1Y**, are sufficient to reconstruct ρ .

5. Discussion

For general n -spin systems, we will just mention some features of the NMR signal and procedure of the density operator reconstruction with a three-spin system. The Hamiltonian is

$$\begin{aligned} \mathcal{H}_3 = & \frac{\omega_1}{2} \sigma_{1z} + \frac{\omega_2}{2} \sigma_{2z} + \frac{\omega_3}{2} \sigma_{3z} \\ & + \frac{\pi}{2} J_{12} \sigma_{1z} \sigma_{2z} + \frac{\pi}{2} J_{13} \sigma_{1z} \sigma_{3z} + \frac{\pi}{2} J_{23} \sigma_{2z} \sigma_{3z}. \end{aligned} \quad (11)$$

From Eq. (1), the NMR signal is composed of 12 components oscillating at frequencies, $\omega_1 \pm \pi J_{12} \pm \pi J_{13}$, $\omega_2 \pm \pi J_{12} \pm \pi J_{23}$, and $\omega_3 \pm \pi J_{13} \pm \pi J_{23}$ and the coefficient of the part varying at frequency $\omega_1 + \pi J_{12} + \pi J_{13}$ is given by

$$\begin{aligned} \text{tr} \{ \rho [& (\sigma_{1x} + \sigma_{1x} \sigma_{2z} + \sigma_{1x} \sigma_{3z} + \sigma_{1x} \sigma_{2z} \sigma_{3z}) \\ & + i (\sigma_{1y} + \sigma_{1y} \sigma_{2z} + \sigma_{1y} \sigma_{3z} + \sigma_{1y} \sigma_{2z} \sigma_{3z})] \}. \end{aligned} \quad (12)$$

Table 1

The relations between the ensemble averages of a quorum of observables in a two-spin system and the 72 quantities measured by a set of nine experiments. The superscript means the unitary operation performed on the density operator and the subscript indicates which spectral line the datum comes from and r and i means real and imaginary parts, respectively

Operator	Formula
σ_{1x}	$\text{avg}(S_{1r}^{11}, S_{2r}^{11}, S_{1r}^{X1}, S_{2r}^{X1}, S_{1r}^{1X}, S_{2r}^{1X}, S_{1r}^{1Y}, S_{2r}^{1Y}, S_{1r}^{XX}, S_{2r}^{XX}, S_{1r}^{XY}, S_{2r}^{XY})$
σ_{1y}	$\text{avg}(S_{1i}^{11}, S_{2i}^{11}, S_{1i}^{Y1}, S_{2i}^{Y1}, S_{1i}^{1X}, S_{2i}^{1X}, S_{1i}^{1Y}, S_{2i}^{1Y}, S_{1i}^{YX}, S_{2i}^{YX}, S_{1i}^{YY}, S_{2i}^{YY})$
σ_{1z}	$\text{avg}(-S_{1i}^{X1}, -S_{2i}^{X1}, S_{1r}^{Y1}, S_{2r}^{Y1}, -S_{1i}^{XX}, -S_{2i}^{XX}, -S_{1i}^{XY}, -S_{2i}^{XY}, S_{1r}^{XX}, S_{2r}^{XX}, S_{1r}^{YY}, S_{2r}^{YY})$
σ_{2x}	$\text{avg}(S_{3r}^{11}, S_{4r}^{11}, S_{3r}^{X1}, S_{4r}^{X1}, S_{3r}^{Y1}, S_{4r}^{Y1}, S_{3r}^{1X}, S_{4r}^{1X}, S_{3r}^{XX}, S_{4r}^{XX}, S_{3r}^{YX}, S_{4r}^{YX})$
σ_{2y}	$\text{avg}(S_{3i}^{11}, S_{4i}^{11}, S_{3i}^{X1}, S_{4i}^{X1}, S_{3i}^{Y1}, S_{4i}^{Y1}, S_{3i}^{1Y}, S_{4i}^{1Y}, S_{3i}^{XX}, S_{4i}^{XX}, S_{3i}^{XY}, S_{4i}^{XY}, S_{3i}^{YY}, S_{4i}^{YY})$
σ_{2z}	$\text{avg}(-S_{3i}^{1X}, -S_{4i}^{1X}, S_{3r}^{1Y}, S_{4r}^{1Y}, -S_{3i}^{XX}, -S_{4i}^{XX}, S_{3r}^{XY}, S_{4r}^{XY}, -S_{3i}^{YY}, -S_{4i}^{YY}, S_{3r}^{YX}, S_{4r}^{YX})$
$\sigma_{1x}\sigma_{2x}$	$\text{avg}(-S_{3r}^{Y1}, S_{4r}^{Y1}, -S_{1r}^{1Y}, S_{2r}^{1Y}, -S_{1r}^{XY}, S_{2r}^{XY}, -S_{3r}^{YX}, S_{4r}^{YX})$
$\sigma_{1x}\sigma_{2y}$	$\text{avg}(-S_{3i}^{Y1}, S_{4i}^{Y1}, S_{1r}^{1X}, -S_{2r}^{1X}, S_{1r}^{XX}, -S_{2r}^{XX}, -S_{3i}^{YY}, S_{4i}^{YY})$
$\sigma_{1x}\sigma_{2z}$	$\text{avg}(S_{1r}^{11}, -S_{2r}^{11}, S_{1r}^{X1}, -S_{2r}^{X1}, S_{3i}^{YX}, -S_{4i}^{YX}, -S_{3r}^{YY}, S_{4r}^{YY})$
$\sigma_{1y}\sigma_{2x}$	$\text{avg}(S_{3r}^{X1}, -S_{4r}^{X1}, -S_{1i}^{1Y}, S_{2i}^{1Y}, S_{3r}^{XX}, -S_{4r}^{XX}, -S_{1i}^{YY}, S_{2i}^{YY})$
$\sigma_{1y}\sigma_{2y}$	$\text{avg}(S_{3i}^{X1}, -S_{4i}^{X1}, S_{1r}^{1X}, -S_{2r}^{1X}, S_{3i}^{XY}, -S_{4i}^{XY}, S_{1r}^{YX}, -S_{2i}^{YX})$
$\sigma_{1y}\sigma_{2z}$	$\text{avg}(S_{1i}^{11}, -S_{2i}^{11}, S_{1i}^{Y1}, -S_{2i}^{Y1}, -S_{3i}^{XX}, S_{4i}^{XX}, S_{3r}^{XY}, -S_{4r}^{XY})$
$\sigma_{1z}\sigma_{2x}$	$\text{avg}(S_{3r}^{11}, -S_{4r}^{11}, S_{3r}^{1X}, -S_{4r}^{1X}, S_{1i}^{XY}, -S_{2i}^{XY}, -S_{1r}^{YY}, S_{2r}^{YY})$
$\sigma_{1z}\sigma_{2y}$	$\text{avg}(S_{3i}^{11}, -S_{4i}^{11}, S_{3i}^{1Y}, -S_{4i}^{1Y}, -S_{1i}^{XX}, S_{2i}^{XX}, S_{1r}^{XY}, -S_{2r}^{XY})$
$\sigma_{1z}\sigma_{2z}$	$\text{avg}(-S_{1i}^{X1}, S_{2i}^{X1}, S_{1r}^{Y1}, -S_{2r}^{Y1}, -S_{1i}^{1X}, S_{2i}^{1X}, S_{1r}^{1Y}, -S_{2r}^{1Y})$

Notice that three-spin product operators $\sigma_{1x}\sigma_{2z}\sigma_{3z}$ and $\sigma_{1y}\sigma_{2z}\sigma_{3z}$ are measured due to the coexistence of two coupling terms $\pi J_{12}2I_{1z}I_{2z}$ and $\pi J_{13}2I_{1z}I_{3z}$ and this makes them possible to get information on the correlation among three spins from NMR spectra and to estimate the density operator. Likewise, in an n -spin system, k -spin product operators ($k \leq n$) can be observed by virtue of $k - 1$ coupling Hamiltonians, and the ensemble averages of $2^{\binom{n-1}{k-1}}$ k -spin product operators can be obtained from each resonance. If the combinations of single spin rotations, which transforms k -spin product operators into k -spin ones, are used to convert the observables, the number of them measured in each experiment does not change. Since there are $3^k \binom{n}{k}$ k -spin product operators, the number of experiments necessary to measure all of them is

$$\left\lceil \frac{3^k \binom{n}{k}}{2n \binom{n-1}{k-1}} \right\rceil = \lceil 3^k / (2k) \rceil.$$

Therefore, we need a set of at least $\lceil 3^n / (2n) \rceil$ experiments for a valid construction of the density operator

but this estimation does not mean that all $4^n - 1$ product operators can be measured with the set of experiments, though the function $3^k / (2k)$ is rapidly increasing with k .

In the above, it was assumed that all spin–spin couplings are resolved but in practice, some coupling Hamiltonians may not be available since they do not exist or are too small to be resolvable. If a spin–spin coupling is missing, the correlations between the two spins involved cannot be obtained by the above method. We need more complicated unitary transforms such as a quantum swap operation to get information on the ensemble averages of those observables and this may inevitably degrade the quality of the measured values. Inversely, some set of unitary transforms can be devised, which allow to measure a quorum of observables in experiments fewer than $3^n / (2n)$, but those operations may lower the accuracy of the density operator due to the inexactness performing them and the decoherence during them.

6. Conclusion

The quantum state tomography on an NMR system was examined by expressing the NMR signal as a composition of the ensemble averages of observables and the case in which all couplings are resolved and the combinations of single spin operations are used to obtain the information was devoted. The approach developed here should help to make clear the origin of the measured quantities and to make easy the establishment of the relation required to the density operator reconstruction in NMR.

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