Efficient Quantum State Tomography for Quantum Information Processing using a
two-dimensional Fourier Transform Technique

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A new method of quantum state tomography for quantum information processing is described.
The method based on two-dimensional Fourier transform technique involves detection of all the off-diagonal elements of the density matrix in a two-dimensional experiment. All the diagonal elements are detected in another one-dimensional experiment. The method is efficient and applicable to a wide range of spin systems. The proposed method is explained using a 2 qubit system and demonstrated by tomographing arbitrary complex density matrices of 2 and 4 qubit systems using simulations.

I. INTRODUCTION

Quantum Computation offers exciting possibilities of solving complex computational problems using algorithms which exploit the quantum nature of the system. The idea, first proposed by Feynman [1], is being feverishly pursued by many [2-6]. Several algorithms like Shor’s factorization algorithm, Grover’s search algorithm, Deutsch-Jozsa algorithm, quantum Fourier transform, quantum counting and quantum error-correction codes have been developed and have clearly established the premise [7-24]. The last step in quantum information processing and quantum simulations is the measurement of the output quantum state, known as quantum state tomography. In the case of ensemble systems this amounts to measuring the output density matrix. The output state of a quantum algorithm normally corresponds to some classical information and therefore, it is sufficient to measure all the diagonal elements of the density matrix which corresponds to the probabilities of various eigenstates. However, full quantum state tomography is generally carried out wherever possible, because of the following reasons; (i) knowledge of the full output density matrix allows one to find out the experimental errors and to calculate the fidelity of the implementation [5,10–14], and (ii) if one wishes to monitor the flow of the implementation of an algorithm at any intermediate step, then the best option is to measure the full intermediate density matrix [11].

For an n-qubit ensemble system, the size of the Hilbert space increases as $2^n$ and the number of density matrix elements increases as $2^n \times 2^n$. Of these there are $M = (2^{n-1})(2^{n-1} + 1)$ independent elements, of which $(n2^{n-1})$ elements are one qubit single quantum observable coherences. To measure the remaining elements, a series of one-dimensional experiments with readout pulses to rotate the unobservables into observables, have been used [10,11,13,14]. Here we propose a new method for
quantum state tomography based on the two-dimensional Fourier transform technique, where all the off-diagonal elements of a density matrix, both unobservable and observable, are measured in a two-dimensional experiment. All the diagonal elements are measured in another one-dimensional experiment.

It has been pointed out [25] that the earlier method of tomography [10] involving a large number of different measurements; while works well for small spin systems, becomes "prohibitively complex" for large spin systems. Such large systems can be easily tomographed using the proposed method. It may be mentioned here, that the proposed method uses a two-dimensional experiment and requires several $t_1$ increments. In principle the size of two-dimensional data is independent of the number of spins (qubits). However, the number of quantus increase linearly with the number of spins. To maintain the same resolution for large number of spins (qubits), the number of $t_1$ increments may have to be increased appropriately (at best linearly). It may be recalled that the same principle is applied to two-dimensional NMR of biomolecules, where the size of data is independent of the size of biomolecules [27]. The proposed method can also be used for tomography in a wider range of spin systems, i.e., quadrupolar or strongly coupled systems, and it requires non-selective r.f. pulses which are devoid of errors caused by the selective pulses used by the earlier method [10]. The method is explained using a 2-qubit system and demonstrated on 2 and 4-qubit systems using simulations.

II. THE METHOD

The method is based on the technique of indirect detection of multiple quantum coherences in NMR spectroscopy by two-dimensional Fourier transform technique [26], wherein all the off-diagonal elements are measured in a two-dimensional experiment (pulse sequence 1(A)). The diagonal elements of the density matrix are measured in another one-dimensional experiment (pulse sequence 1(B)). The NMR pulse sequences for the two experiments are,

\[(A) \ t_1 - (\pi/2)_y - G_z - \alpha_y - \text{detect}(t_2),\]
\[(B) \ G_z - \beta_y - \text{detect}(t_2),\]

where $t_1$ and $t_2$ are the variable time periods of system evolution, $(\pi/2)_y$, $\alpha_y$ and $\beta_y$ are the rf pulses, and $G_z$ is the field-gradient pulse.

In experiment 1(A), a given density matrix $\sigma(0)$ is allowed to evolve for a time $t_1$, at the end of which a $(\pi/2)_y$ pulse transform every element into all other elements of the density matrix, including diagonal elements. The $G_z$ pulse dephases the off-diagonal elements averaging them to

...
zero, and retains only the diagonal elements. A $\alpha_{-y}$ pulse transforms the diagonal elements into all elements of the density matrix including single qubit single quantum coherences. These single quantum coherences are then detected as a function of time variable $t_2$. A series of experiments are performed by systematic increment of the $t_1$ period and the collected two-dimensional time domain data set $s(t_1, t_2)$ is double Fourier transformed yielding a two-dimensional frequency domain spectrum $S(\Omega_1, \Omega_2)$. $S(\Omega_1, \Omega_2)$ contains along $\Omega_2$ all single qubit single quantum coherences and along $\Omega_1$, contribution of every off-diagonal elements of the density matrix to these transitions, dispersed and displayed by their specific frequency of evolution in the time-domain $t_1$. Cross-sections parallel to $\Omega_1$ at one single quantum resonance frequency can be fitted to $\sigma(0)$, yielding all the off-diagonal elements in single two-dimensional experiment. The diagonal elements of $\sigma(0)$ do not contribute to the spectrum.

To obtain the diagonal elements; experiment 1(B) begins by destroying all off-diagonal elements of $\sigma(0)$ by a gradient pulse, then using a small angle detection pulse to convert difference in diagonal elements into observable one qubit single quantum coherences by linear response. The amplitudes of the coherences allow calculation of all the off-diagonal elements. The above protocol is explained in the following by explicit calculations on a two qubit system.

III. TWO QUBIT SYSTEM

Consider a two qubit system consisting of two spin 1/2 nuclei of Larmor frequencies $\omega_1$ and $\omega_2$, coupled by a weak indirect coupling $J$. The Hamiltonian for the system is, $H = \omega_1 I_{1z} + \omega_2 I_{2z} + J I_{1z} I_{2z}$, where $I_{jz}$ ($j = 1, 2$) are the spin operators. A selective rf pulse of angle $\theta$ and phase $\phi$ on-resonance on spin $j$ corresponds to a unitary transform, $U^j_{\theta, \phi} = \exp\{-i\theta(I_{jx}\sin\phi + I_{jy}\cos\phi)\}$. All quantum algorithms are implemented in NMR by a specific pulse sequence involving the evolutions under system Hamiltonian and rf pulses. A general Hermitian complex trace-less deviation density matrix for 2 qubits, has 15 independent elements, is spanned by 15 product operators $[27]$, and can be expressed as:

$$\sigma(0) = \sum_{k,l} q_{kl} I_{1k} I_{2l}, \quad (2)$$

where $k$ and $l$ can take values 0,1,2,3 corresponding to $o, x, y, z$ respectively, but not simultaneously 0, and $I_{1o} = I_{2o} = I$ is unit matrix, and $q_{kl}$ are real coefficients. All the elements of the density matrix $\sigma(0)$ can be classified into two groups: (i) diagonal elements involving the deviation populations $\Delta P_k$ (deviations from an average population) of various eigenstates and (ii) off-diagonal elements

$$\Delta P_k = \sum_{kl} q_{kl} I_{1k} I_{2l}.$$
involving one-qubit coherences (1Q elements) and multi-qubit coherences (zero and double quantum elements for a 2 qubit system).

\[
\sigma(0) = \begin{pmatrix}
\Delta P_1 & 1Q_1 & 1Q_2 & 2Q_2 \\
1Q_1^* & \Delta P_3 & 2Q_0 & 1Q_3 \\
1Q_2^* & 2Q_0^* & \Delta P_3 & 1Q_4 \\
2Q_2^* & 1Q_3^* & 1Q_4^* & \Delta P_4
\end{pmatrix}.
\]

The trace condition \(\sum_k \Delta P_k = 0\) yields 15 independent (12 off-diagonal and 3 diagonal) elements in this case. Each 1Q element, known as a single quantum element, corresponds to product operators of the type \(I_{1x}, I_{1y}, I_{1x}I_{2z}, I_{1y}I_{2z}\), and \(I_{2x}, I_{2y}, I_{2x}I_{1z}\), and \(I_{2y}I_{1z}\). Each 2Q element, known as zero or double quantum element depending on the frequency of evolution \(\omega_1 - \omega_2\) or \(\omega_1 + \omega_2\), corresponds to an expansion in terms of \(I_{1x}I_{2x}, I_{1x}I_{2y}, I_{1y}I_{2x}\) and \(I_{1y}I_{2y}\).

**A. Measurement of off-diagonal elements**

Effect of the pulse sequence 1(A) on any initial density matrix \(\sigma(0)\) can be described as [27],

\[
\begin{align*}
\sigma(0) & \xrightarrow{t_1} \sigma_1(t_1) = e^{-i\mathcal{H}_1} \sigma(0) e^{i\mathcal{H}_1} \\
& \xrightarrow{(\frac{\pi}{2})} \sigma_2(t_1) = e^{-i(I_{1y}+I_{2y})\pi/2} \sigma_1(t_1) e^{i(I_{1y}+I_{2y})\pi/2} \\
& \xrightarrow{G_z} \sigma_3(t_1) = \mathcal{P} \sigma_2(t_1) \\
& \xrightarrow{\alpha} \sigma_4(t_1) = e^{i(I_{1y}+I_{2y})\alpha} \sigma_3(t_1) e^{-i(I_{1y}+I_{2y})\alpha} \\
& \xrightarrow{t_2(measure)} \sigma_5(t_1, t_2) = e^{-i\mathcal{H}_2} \sigma_4(t_1) e^{i\mathcal{H}_2}.
\end{align*}
\]

Here the operator \(\mathcal{P}\) projects and retains only the diagonal part of \(\sigma_2(t_1)\). The complex time domain signal \(s(t_1, t_2)\) obtained on measurement as a function of \(t_2\), is \(s(t_1, t_2) = \text{Trace}[(I_1^++I_2^+)\cdot\sigma_5(t_1, t_2)]\), which after double Fourier transform gives two-dimensional (2D) spectrum \(S(\Omega_1, \Omega_2)\) which is a function of the two frequency variables \(\Omega_1\) and \(\Omega_2\). The \(\Omega_2\) axis of this spectrum has only the single quantum (1Q) elements (four transitions in the 2-qubit system). Along the \(\Omega_1\) axis of the 2D spectrum all the off-diagonal elements of \(\sigma(0)\) yield peaks corresponding to their amplitudes \((q_{kl})\) and individual evolution frequencies during the time period \(t_1\).

Cross-sections of the signal after Fourier Transform with respect to \(t_2\), but before \(t_1\), \([S(t_1, \Omega_1)]\) taken parallel to \(t_1\) at \(\Omega_2 = \omega_1^+\) and \(\Omega_2 = \omega_2^+\) respectively correspond to,

\[
\sigma_4(\omega_1^+) = e^{-t_1/T_2} \sin\alpha[(q_{10} + q_{13})\cos(\omega_1^+ t_1) + (q_{10} - q_{13})\cos(\omega_1^- t_1)]
\]
one obtains the two-dimensional (2D) spectrum $S_T$ in Eq. (2), and
higher-qubit coherences, appropriate values of various orders [28].

and the sine terms dispersive Lorenztian lines. All the coefficients of off-diagonal elements of
each coherence, but taken identical here for simplicity. On $t$ can be obtained by fitting the cross-sections from the two-dimens
$\sigma$ the 2-qubit density matrix
Two cross-sections, one at each qubit, are sufficient to calculate all the off-diagonal elements of
1 parallel to $\Omega_1(A)$. Similarly the undesired ‘axial peaks’ (having zero frequency during
diagonal elements do not interfere with the two-dimensional spectrum obtained by pulse sequence
the remaining cross-sections can be used to minimise the errors. It may also be noted that the
longitudinal relaxations during $t_1$ period) arising due to
the longitudinal relaxations during $t_1$ period [27] are also suppressed by the present scheme.

In the two-qubit case, the one-qubit and two-qubit coherences have different conversion ratios,
namely, $\sin\alpha$ and $\frac{1}{2}\sin2\alpha$. As a compromise $\alpha = \pi/4$ has been used here. For qubit systems having
higher-qubit coherences, appropriate values of $\alpha$ should be used which optimizes the intensities of
various orders [28].

B. Measurement of diagonal elements

The transformations of the density matrix $\sigma(0)$ by the pulse sequence 1(B) are as follows.

$$\sigma(0) \xrightarrow{G_z} q_{30}I_{1z} + q_{03}I_{2z} + q_{33}I_{1z}I_{2z}$$
$$\xrightarrow{\beta_z} q_{30}(I_{1z}\cos\beta + I_{1z}\sin\beta) + q_{03}(I_{2z}\cos\beta + I_{2z}\sin\beta)$$
\[ q_{33}(I_{1z}\cos\beta + I_{1x}\sin\beta)(I_{2z}\cos\beta + I_{2x}\sin\beta) \]
\[
\to \text{Measure.} \quad (6)
\]

To measure the coefficients under linear response, \( \beta \) should be small [27]. The measured one-qubit coherences then are

\[ \beta [q_{30}I_{1x} + q_{03}I_{2x} + q_{33}(I_{1x}I_{2z} + I_{1z}I_{2x})], \quad (7) \]

which can be rearranged as,

\[ \beta [(q_{30} + q_{33}/2)(I_{1x} + 2I_{1z}I_{2x}) + (q_{30} - q_{33}/2)(I_{1x} - 2I_{1z}I_{2x}) + (q_{03} + q_{33}/2)(I_{2x} + 2I_{1z}I_{2x}) + (q_{03} - q_{33}/2)(I_{2x} - 2I_{1z}I_{2x})]/2. \quad (8) \]

The coefficients of the four terms in the above expression are proportional to the intensities of the corresponding four transitions of a two qubit system. After calculating \( q_{30}, q_{03}, \) and \( q_{33}, \) all the diagonal elements of the density matrix \( \sigma(0) \) can be calculated, since the diagonal part is equal to \( q_{30}I_{1z} + q_{03}I_{2z} + q_{33}I_{1z}I_{2z}. \)

It should be noted that the gradient pulse \( G_z \) used in pulse sequences 1(A) to destroy off-diagonal elements, does not destroy homonuclear zero-quantum coherences. In such cases, an extra small delay \( \tau_m \) along with \( G_z, \) randomly varied between each \( t_1 \) experiment can suppress the homonuclear zero quantum coherence [27]. In experiment 1(B), signal averaging using a few randomly varied \( \tau_m \) along with \( G_z \) would suppress the homonuclear zero quantum coherences.

The above schemes 1(A) and (B) assume ideal r.f. pulses. To correct for errors due to imperfection of the r.f. pulses a third one dimensional experiment can be performed to measure the one qubit coherences directly without application of any pulses. These coherences can then be used to normalize all other elements of the density matrix measured by experiments 1(A) and (B).

**IV. SIMULATION**

To demonstrate the protocol we tomograph an arbitrary complex density matrix with simulations. In a 2-qubit system, such a density matrix is of the form;

\[
\sigma(0) = I_{1z} + 2.3I_{2z} + 6.7I_{1z}I_{2z} + I_{1x} + 10I_{1x}I_{2x} + 5I_{1y} + 3.5I_{1y}I_{2y} + 2.5I_{1y}I_{2y} + 7.2I_{1y}I_{1z} + 13I_{1x}I_{2x} + 1.45I_{1x}I_{2y} + 2I_{2x} + 3.45I_{1z}I_{2x} + 6.9I_{2y} + 6.753I_{1z}I_{2y}
\]
We assume the Larmor frequencies of the two qubits (spins) as \( \omega_1=1200 \text{ Hz} \), \( \omega_2=1800 \text{ Hz} \) and the indirect coupling constant between the qubits as \( J=200 \text{ Hz} \). Experiment 1(A) is performed to obtain all the off-diagonal elements. \( \alpha \) was chosen as \( 45^\circ \). 512 \( t_1 \) increments were performed yielding the 2D spectrum shown in Fig. 1(a). Cross sections parallel to \( \Omega_1 \) taken at one of the transitions of each qubit are shown in Fig 1(b) and (c). These cross sections were fitted to get all the complex off-diagonal elements of the density matrix. \( T_2 \) was taken as 10ms for all coherences. The diagonal elements were mapped using experiment 1(B) with \( \beta = 10^\circ \), Fig 1(d). The real and imaginary parts of the tomographed density matrix are shown respectively in Figs. 1(e) and 1(f). The calculated density matrix matches the input density matrix better than 0.01% for all complex elements. We have also carried out the simulations on a 4-qubit system (Fig. 2) and tomographed the density matrix with 99.7% fidelity.

V. CONCLUSION

Two-dimensional nuclear magnetic resonance spectroscopy provides an efficient method for the quantum state tomography. Only an one-dimensional and a two-dimensional experiment are required for measuring all the elements of the density matrix. Since the earlier method requires a series of one dimensional experiments with different readout pulses, for large spin systems the approach becomes enormously complex [16]. However such systems can easily be tomographed using the proposed method by aptly increasing the \( t_1 \) increments. The earlier method uses spin-selective r.f. pulses, which requires long-duration irradiation of a particular spin. During such a pulse, the unperturbed spins evolve under the Zeeman and coupling interactions, introducing errors due to measurement [15,16]. The method described here requires non-selective short-duration r.f. pulses which do not introduce such errors. Search of more qubits has led researchers to use strongly coupled spin-1/2 nuclei and quadrupolar nuclei (spin>1/2) oriented in liquid crystalline matrices [19–23]. For such systems the notion of spin-selectivity does not apply, but the proposed method based on non-selective pulses can be used for tomography. Recently, the method was used to tomograph the states while quantum information processing in weakly and strongly coupled spin systems [23,24]. This method can also be extended to a 3-dimensional experiment in which quanta of various orders are displaced...
in different planes of the 3-D experiment, increasing the detectibility and the resolution of the spectrum [29].

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FIG. 1. Tomography of a complex density matrix in a 2 qubit system. (a) is the 2D spectrum generated by experiment 1(A) for tomography of all off diagonal elements. (b) is the cross section parallel to $\Omega_1$ taken at $\Omega_2 = 1300$ Hz ($\omega_1 + J/2$) (a transition frequency of first qubit), (c) is the cross section parallel to $\Omega_1$ taken at $\Omega_2 = 1900$ Hz ($\omega_2 + J/2$) (a transition frequency of the second qubit) and (d) is the 1D spectrum obtained by experiment of 1(B) for mapping all diagonal elements of $\sigma(0)$. (e) and (f) are the real and imaginary part of the tomographed density matrix. The calculated values of the tomographed matrix are $\sigma_{11} = 3.2501$, $\sigma_{12} = 1.8625 - 5.1385i$, $\sigma_{13} = 3.0001 - 3.375i$, $\sigma_{14} = 2.6501 - 2.1624i$, $\sigma_{21} = 1.8625 + 5.1385i$, $\sigma_{22} = -2.3251$, $\sigma_{23} = 3.8750 + 1.4374i$, $\sigma_{24} = -2.0001 - 1.625i$, $\sigma_{31} = 3.0001 + 3.375i$, $\sigma_{32} = 3.8750 - 1.4374i$, $\sigma_{33} = -1.025$, $\sigma_{34} = 0.1376 - 1.7618i$, $\sigma_{41} = 2.6501 + 2.1624i$, $\sigma_{42} = -2.0001 + 1.625i$, $\sigma_{43} = 0.1376 + 1.7618i$, and $\sigma_{44} = 0.025$. 
FIG 2. Tomography of a complex density matrix in 4-qubit system. An arbitrary complex density matrix \( \sigma(0) = 0.8I_{1x} + I_{1y} + 0.5I_{2x} + I_{2y} + 0.9I_{3x} + 1.1I_{3y} + I_{4x} + 1.2I_{4y} + 6.3I_{1x}I_{2x}I_{3x}I_{4x} + 3.9I_{1x}I_{2y}I_{3y}I_{4y} + I_{1x}I_{2y}I_{3x}I_{4x} + 1.3I_{2x}I_{3x}I_{4x} + 1.9I_{1x}I_{2x}I_{3y} + 1.5I_{1x}I_{2y}I_{3y}I_{4x} + 0.6I_{4x} + I_{2x}I_{4x} + 1.3I_{2x}I_{3x}I_{4x} + 2I_{1x}I_{2x}I_{3x}I_{4x} \), is reconstructed with the 2D Fourier Transform technique. The frequencies and couplings used in the simulation are \( \omega_1 = 600Hz, \omega_2 = 750Hz, \omega_3 = 1000Hz, \omega_4 = 1400Hz, J_{12} = 20Hz, J_{13} = 10Hz, J_{14} = 70Hz, J_{23} = 35Hz, J_{24} = 24Hz \) and \( J_{34} = 16Hz \). (a) Shows the real part of \( \sigma(0) \), (b) is the real part of reconstructed density matrix and (c) the differences ( magnified by \( 10^3 \)) between the elements of (a) and (b). The 256 complex elements of \( \sigma(0) \) (imaginary part not shown here) were tomographed with more than 99.7% accuracy.