Analysis of density matrix reconstruction in NMR quantum computing

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Abstract
Reconstruction of density matrices is important in NMR quantum
computing. An analysis is made for a 2-qubit system using the error matrix
method. It is found that the state tomography method determines well the
parameters that are necessary for reconstructing the density matrix in NMR
quantum computations. Analysis is also made for a simplified state
tomography procedure that uses fewer read-outs. The result of this analysis
with the error matrix method demonstrates that a satisfactory accuracy in the
density matrix reconstruction can be achieved even in a measurement with
the number of read-outs being largely reduced.

Keywords: State tomography, density matrix reconstruction, NMR quantum
computing

1. Introduction

The study of quantum computers has attracted considerable attention since 1994 when Shor introduced a quantum mechanical algorithm for efficient factoring of large numbers [1]. In another remarkable work in 1996, Grover discovered that quantum mechanics can help to speed up data search in an unsorted database [2,3]. Quantum mechanics that, for nearly a century, has been a basic tool for understanding the microscopic world is becoming a powerful new weapon for computation, communication and information processing.

Realizing quantum computing experimentally has sparked an explosion of interest. NMR quantum computation is particularly attractive among many proposed physical systems to implement quantum computation, such as trapped ions, optical photons, quantum dots and so on, because nuclear spins are extremely well isolated from their environment and readily manipulated with modern NMR techniques. Comprehensive algorithm realizations have been accomplished for the Deutsch–Jozsa algorithm in 2-qubit and 3-qubit systems [4–6] and a 5-qubit system [7], and for Grover's algorithm with 2-qubit [8, 9] and 3-qubit systems [10]. The order-finding problem in a 5-qubit system has recently been demonstrated in NMR [11], and a Cat state is prepared in a 7-qubit system [12].

The fundamental elements for information processing in NMR are two-level nuclear spins that are bound together in a single molecule. Introduced in 1997 by Cory *et al* [13] and Gershenfeld *et al* [14], the NMR scheme uses bulk numbers of molecules. The NMR techniques cannot control the quantum states of individual molecules; instead, all the molecules in the sample are manipulated in parallel. In fact, a liquid NMR sample is initially in thermal equilibrium at room temperature. The directions of the nuclear spins have a Boltzman distribution and are not polarized along the strong magnetic field.

Reconstruction of the quantum state, or quantum state tomography, is not only important in quantum computation, but is also important for general purposes. It has attracted many investigations. For instance, the discrete Wigner function has been used to infer the quantum states of finite-dimensional systems from measurements by Leonhardt [15, 16]. Walser *et al* [17] have proposed a scheme to reconstruct the state of a single quantized cavity mode. Amiet and Weigert [18–20] have

studied various aspects of reconstruction of the density matrix for a spin state in pure or mixed states. Reconstruction of the state of light has been extensively studied by Leonhardt [21].

In NMR quantum computation, the liquid ensemble is described by the density matrix. The state of the NMR computer can be obtained by the state-tomography technique [22]. In order to extract the density matrix, for example, for a 2-qubit system, 18 read-outs have to be performed. In general, for an n-qubit system, construction of the density matrix requires $3^n \times n$ read-outs. After signal read-out, the area of the spectrum is integrated and the density matrix is reconstructed through numerical methods. Obviously, the amount of work in experiment and post-processing is huge when n becomes moderately large.

In this paper we study the reconstruction of the density matrix in NMR. The mathematical structures of the density matrix reconstruction is analysed. We found that the full state tomography read-outs, which consist of 18 read-outs for a 2-qubit system, is well conditioned. However, a smaller number of read-outs can also determine the density matrix well. We compared the results of the 2-qubit density matrix in the NMR experiment with the full read-outs and much reduced read-outs respectively, and found that they agree with the theoretical analysis.

The paper is organized as follows. In section 2 we describe the procedures to construct the density matrix. We analyse the density matrix reconstruction procedure in section 3. In section 4 we discuss the reduction of the number of read-outs in constructing the density matrix. We apply the analysis to a 2-qubit NMR experiment and the results indicate that it is possible to construct a density matrix with a much reduced number of read-outs and at the same the loss of accuracy is small. Finally in section 5 we give a summary.

2. Reconstruction of the density matrix

In an NMR measurement, each read-out pulse can only give some off-diagonal matrix elements of the density matrix. To obtain the rest of the matrix elements, one has to rotate the original density matrix through rotational operations. In a 2-qubit system, in order to construct the density matrix, one needs to perform the following operations [22]: II, IX, IY, XI, XX, XY, YI, YX and YY. Here, I, X and Y stand for, respectively, the identity operation, a 90° rotation about the x-axis, and a 90° rotation about the y-axis. Thus, in a state tomography, these operations are performed before NMR read-out measurements. We explain this using an example below.

Suppose that we use the nuclear spins of H and P in a phosphorous acid as our qubits. Since for a usual NMR system, only one nuclear spin can be measured at a time, we have to perform the measurement separately for the two nuclear spins. We first start a computation and do a measurement on H at the required stage. We then restart the computation from the beginning and measure the signal corresponding to P. Next, we restart the computation, but this time perform the operation IX at the required stage before measuring the signal. This process is carried out separately for H and P nuclear spins, and the nine operations are successively performed for each of them. This means that we have to perform a total of $9 \times 2 = 18$ read-outs.

Taking $|\uparrow\rangle = |1\rangle$ and $|\downarrow\rangle = |0\rangle$, the matrices of the nine operations are

$$II = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$IX = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ 0 & 0 & -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix},$$

$$IY = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix},$$

$$XI = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{i}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{bmatrix},$$

$$XX = \begin{bmatrix} \frac{1}{2} & -\frac{i}{2} & -\frac{i}{2} & -\frac{1}{2} \\ -\frac{i}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{i}{2} \\ -\frac{i}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{i}{2} \\ -\frac{1}{2} & -\frac{i}{2} & -\frac{i}{2} & \frac{1}{2} \end{bmatrix},$$

$$XY = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{i}{2} & \frac{i}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{i}{2} & -\frac{i}{2} \\ -\frac{i}{2} & -\frac{i}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{i}{2} & -\frac{i}{2} & -\frac{1}{2} & \frac{1}{2} \end{bmatrix},$$

$$YI = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{bmatrix},$$

$$YX = \begin{bmatrix} \frac{1}{2} & -\frac{i}{2} & \frac{1}{2} & -\frac{i}{2} \\ -\frac{i}{2} & \frac{1}{2} & -\frac{i}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{i}{2} & \frac{1}{2} & -\frac{i}{2} \\ \frac{i}{2} & -\frac{1}{2} & -\frac{i}{2} & \frac{1}{2} \end{bmatrix},$$

$$YY = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}.$$

(1)

Let us assume that the density matrix of the system takes the form

$$\rho = \begin{bmatrix} \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{12}^* & \rho_{22} & \rho_{23} & \rho_{24} \\ \rho_{13}^* & \rho_{23}^* & \rho_{33} & \rho_{34} \\ \rho_{14}^* & \rho_{24}^* & \rho_{34}^* & \rho_{44} \end{bmatrix}$$

$$= \begin{bmatrix} x_1 & x_2 + ix_{11} & x_3 + ix_{12} & x_4 + ix_{13} \\ x_2 - ix_{11} & x_5 & x_6 + ix_{14} & x_7 + ix_{15} \\ x_3 - ix_{12} & x_6 - ix_{14} & x_8 & x_9 + ix_{16} \\ x_4 - ix_{13} & x_7 - ix_{15} & x_9 - ix_{16} & x_{10} \end{bmatrix}.$$

(2)

The NMR read-out signal can only give $x_2 + ix_{11}$ and $x_9 + ix_{16}$ for the nuclear spin of P, and $x_3 + ix_{12}$ and $x_7 + ix_{15}$ for the nuclear spin of H. For example, the element ρ_{13} in equation (2)

corresponds to the left peak of the spectrum of H, while the element ρ_{24} to the right peak of it. Similarly, the element ρ_{12} corresponds to the left peak of the spectrum of P, and the element ρ_{34} to the right peak of the same spectrum. To obtain other elements in the density matrix, we have to perform one of the nine operations for the system so that the desired elements are transformed to the positions labelled as 12, 13, 24 and 34 in the density matrix, and can thus be measured. The read-out gives the elements ρ'_{12}, ρ'_{13} and ρ'_{24}, ρ'_{34} in the rotated density matrix. These rotated matrix elements are linear combinations of the original matrix elements. For each of the nine operations, one makes two measurements for the nuclear spins of H and P, and each measurement provides two matrix elements which contains a real and an imaginary part. Altogether, we finally obtain $4 \times 9 \times 2 = 72$ equations with 16 unknowns.

The coefficients in these equations form a matrix with a size of 72×16. The rank of this coefficient matrix is only 15 since the matrix can be added with a matrix of a constant times the unit matrix without changing the results. In practice, we can add one more equation by letting the trace of the density matrix be 1 after normalizing the integrations of the spectrum. Thus, in total we have 73 equations. To determine the elements in the density matrix, one needs to solve the following set of linear equations for x_i:

$$\sum_{i=1}^{16} A_{\alpha i} x_i = B_\alpha, \qquad \{\alpha = 1, 2, \ldots, 3\}, \qquad (3)$$

where $A_{\alpha i}$ is the coefficient of x_i in the αth equation and it varies with read-out for different rotations, and B_α is the integrated area of the spectrum. There are certainly redundant expressions in (3) since the number of equations is more than the number of unknowns. The standard way of dealing with this problem is to use the least-square-fitting procedure that is widely used in various problems in science and engineering. We minimize the quantity χ^2 defined as

$$\chi^2 = \sum_\alpha \left(\sum_{i=1}^{16} A_{\alpha i} x_i - B_\alpha \right)^2. \qquad (4)$$

To find the minimum, we carry out a variation procedure on χ^2 with respect to all parameters, which gives

$$\sum_{j=1}^{16} C_{ij} x_j = b_i, \qquad (5)$$

where

$$C_{ij} = \sum_\alpha A_{\alpha i} A_{\alpha j}, \qquad \text{and} \qquad b_i = \sum_\alpha B_\alpha A_{\alpha i}. \qquad (6)$$

The number of equations in (5) is now equal to the number of unknowns. These linear equations can be solved by standard numerical method such as the Gaussian elimination. In principle, such problems can be solved in this way. However, in most of our cases, not every parameter can be experimentally well determined. In the least-square-fitting procedure, these less well-determined matrix elements might possibly bring spurious values into the numerical calculation while leaving the χ^2 value small. In other words, the χ^2 might not be very sensitive in response to a large variation in experiment.

For instance, if we have a set of equations, $x + y = e1$, $x + 1.001y = e2$, this set of equations determines the sum of x and y very well, and the difference between x and y is poorly determined. The χ^2 is insensitive to a change in $x - y$ while leaving $x + y$ unchanged.

3. An analysis of the density matrix reconstruction

In order to obtain the density matrix, one needs to use the least-square-fitting method [23] to derive them from the experimental data. Similar problems actually occur in other fields of science as well. Here, we adopt a variant of the least-square-fitting method from nuclear physics to solve the problem. In the large-scale nuclear shell model calculations, Wildenthal *et al* [24] employed the error matrix method to analyse the sensitivity of the nuclear structure to experimental input. In their method, instead of solving equation (3) directly, one first solves the eigenvalue problem for C defined in (6),

$$UCU^+ = C_d. \qquad (7)$$

Here, U is the unitary matrix that diagonalizes C. C_d is called the error matrix [24]. Then equation (3) becomes

$$C_d y = b', \qquad (8)$$

where $y_i = U_{ij}x_j$ and $b'_i = U_{ij}b_j$. b'_i contains experimental information. Since C_d is diagonal, we can determine y_i by

$$y_i = \frac{b'_i}{(C_d)_{ii}}. \qquad (9)$$

b'_i contains experimental uncertainties, and any change in b'_i will cause y_i to change. However, if the diagonal matrix element $(C_d)_{ii}$ is large (say, of the order of 1), y_i will be insensitive to changes in b'_i, and thus it can be well determined. Conversely, a small $(C_D)_{ii}$ (say, 0.001) means that the corresponding y_i is very sensitive to experiment, and any small variation in b' will cause a large change in y. In this case, y is not well determined, and special effort is necessary to ensure that b' is sufficiently accurate. If this is not possible, then during the fitting process, the y' that corresponds to small eigenvalues of C will be kept constant by physical considerations. In nuclear structure studies, the critical constant value was chosen as 0.001.

The C matrix for a 2-qubit system with all the nine transformations performed (with 18 read-outs, and 73 linear equations) is

$$C = \begin{bmatrix} 3 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 5 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 5 \end{bmatrix}.$$

$$(10)$$

Solving the eigenvalue problem, and we obtain the 16 eigenvalues of C. They are: 4, 4, 4, 4, 4, 6, 6, 3, 3, 2, 6, 4, 4, 4, 4, 6. The y are the combinations of the x coefficients

$$y_1 = -0.37x_3 + 0.82x_4 - 0.24x_6;$$

$$y_2 = -0.19x_1 + 0.41x_2 - 0.17x_3 - 0.32x_4 - 0.19x_5$$
$$\quad -0.59x_6 + 0.17x_7 - 0.19x_8 - 0.41x_9 - 0.19x_{10};$$

$$y_3 = -0.0087x_1 - 0.093x_2 - 0.57x_3 - 0.39x_4 - 0.0087x_5$$
$$\quad +0.42x_6 + 0.57x_7 - 0.0087x_8 + 0.093x_9 - 0.0087x_{10};$$

$$y_4 = 0.30x_1 - 0.30x_2 - 0.093x_3 - 0.26x_4 + 0.30x_5$$
$$\quad -0.61x_6 + 0.093x_7 + 0.30x_8 + 0.30x_9 + 0.30x_{10};$$

$$y_5 = -0.35x_1 - 0.48x_2 + 0.027x_3 - 0.035x_4 - 0.35x_5$$
$$\quad -0.20x_6 - 0.027x_7 - 0.35x_8 + 0.48x_9 - 0.35x_{10};$$

$$y_6 = -0.55x_2 + 0.44x_3 + 0.44x_7 - 0.55x_9;$$

$$y_7 = -0.44x_2 - 0.55x_3 - 0.55x_7 - 0.44x_9;$$

$$y_8 = 0.71x_5 - 0.71x_8;$$

$$y_9 = -0.71x_1 + 0.71x_{10};$$

$$y_{10} = 0.50x_1 - 0.50x_5 - 0.50x_8 + 0.50x_{10};$$

$$y_{11} = 0.71x_{12} + 0.71x_{15};$$

$$y_{12} = -0.71x_{12} + 0.71x_{15};$$

$$y_{13} = x_{13};$$

$$y_{14} = x_{14};$$

$$y_{15} = 0.71x_{11} - 0.71x_{16};$$

$$y_{16} = 0.71x_{11} + 0.71x_{16}.$$

Some of the y are directly the x parameters in the density matrix such as y_{13} and y_{14}, and others are combinations of the x parameters. They are all well determined by the experimental data.

4. Reduction of experimental read-outs

In the process of the density matrix reconstruction discussed above, each signal read-out provides us two equations. By performing all nine operations for P and H, and the normalization condition, we have 73 equations. However, these equations are over-determined. The question is if it is possible to determine the density matrix with less read-outs. It will be very interesting to see what is the minimum number of operations to determine the density matrix without loss of much accuracy. Intuitively, we may think about four read-outs because there are altogether 16 unknowns. However, a detailed analysis of the rank of equations indicated that any four read-outs combined together cannot provide sufficient numbers of independent equations. The minimum number of read-outs to be performed is five. In table 1 we give the various set of five read-outs. In the table, operation 1 is the II with H signal acquisition (see caption for details). From the table we see that no arbitrary combination of five operations are possible.

To see how well the density matrix is determined by a smaller number of read-outs, we choose a six read-out case. The six read-outs are: II, IX, IY, XX for one of the nuclear spins (H) and II, IX for the other (P). In this situation, the corresponding C matrix becomes

$$C = \begin{bmatrix}
\frac{11}{8} & 0 & 0 & 0 & \frac{7}{8} & 0 & 0 & \frac{7}{8} & 0 & \frac{7}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{5}{2} & 0 & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{7}{8} & 0 & 0 & 0 & \frac{11}{8} & 0 & 0 & \frac{7}{8} & 0 & \frac{7}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{3}{2} & 0 & 0 & 0 & \frac{5}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{7}{8} & 0 & 0 & 0 & \frac{7}{8} & 0 & 0 & \frac{3}{8} & 0 & \frac{7}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{7}{8} & 0 & 0 & 0 & \frac{7}{8} & 0 & 0 & \frac{7}{8} & 0 & \frac{11}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 & 0 & -\frac{1}{2} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{3}{2} & -\frac{1}{2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & \frac{3}{2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & \frac{3}{2}
\end{bmatrix}. \tag{11}$$

The eigenvalues of the C matrix are: 1, 2, 1, $\frac{1}{2}$, $\frac{1}{2}$, 1, 4, 2, 4, $\frac{1}{2}$, 1, 3, 1, 2, 1, 2. It can be seen that the eigenvalues are all quite large. The y expressions corresponding to the eigenvalues are

$$y_1 = -x_6$$

$$y_2 = x_2;$$

$$y_3 = x_4;$$

$$y_4 = -0.79x_1 + 0.21x_5 + 0.58x_8;$$

$$y_5 = -0.21x_1 + 0.79x_5 - 0.58x_8;$$

$$y_6 = 0.71x_3 - 0.71x_7;$$

$$y_7 = 0.71x_3 + 0.71x_7;$$

$$y_8 = x_9;$$

$$y_9 = -0.50x_1 - 0.50x_5 - 0.50x_8 - 0.50x_{10}; \tag{12}$$

$$y_{10} = -0.29x_1 - 0.29x_5 - 0.29x_8 + 0.87x_{10};$$

$$y_{11} = -0.71x_{12} + 0.71x_{15};$$

$$y_{12} = 0.71x_{12} + 0.71x_{15};$$

$$y_{13} = -0.71x_{13} - 0.71x_{14};$$

$$y_{14} = -0.71x_{13} + 0.71x_{14};$$

$$y_{15} = -0.71x_{11} - 0.71x_{16};$$

$$y_{16} = -0.71x_{11} + 0.71x_{16}.$$

The density matrix elements are also determined as the ones with 18 read-outs. However, the saving in the number of read-outs is great ($18 - 6 = 12$). Because we have less read-outs now, the statistics in this case is surely poorer, and this will reduce the accuracy of the parameters determined. Nevertheless, because of the intrinsic mathematical structure, the uncertainties in the experimental data affect the parameters insensitively, and the loss in accuracy is not very big.

As an example, we have analysed the density matrix for a 2-qubit system in an NMR experiment [26]. The theoretical prediction of the density matrix is

$$\rho_{th} = \begin{bmatrix}
0.31 & 0.31 & 0.31 & -0.063 - 0.13i \\
0.31 & 0.31 & 0.31 & -0.063 - 0.13i \\
0.31 & 0.31 & 0.31 & -0.063 - 0.13i \\
-0.063 + 0.13i & -0.063 + 0.13i & -0.063 + 0.13i & 0.063
\end{bmatrix}. \tag{13}$$

When constructing the density matrix using all 73 equations, we obtain

$$\rho_{all} = \begin{bmatrix}
0.36 & 0.33 - 0.087i & 0.31 + 0.037i & -0.034 - 0.22i \\
0.33 + 0.087i & 0.30 & 0.28 - 0.022i & -0.079 - 0.14i \\
0.31 - 0.037i & 0.28 + 0.022i & 0.23 & -0.044 - 0.13i \\
-0.034 + 0.22i & -0.079 + 0.14i & -0.044 + 0.13i & 0.12
\end{bmatrix}. \tag{14}$$

If we take only 49 equations out of the 73 equations, which means that we take only 12 read-outs (which contains all nine

Table 1. Minimum set of read-outs combinations. Here $1 = II$, $2 = IX$, $3 = IY$, $4 = XI$, $5 = XX$, $6 = XY$, $7 = YI$, $8 = YX$, $9 = YY$ with H signal acquisition, and $10 = II$, $11 = IX$, $12 = IY$, $13 = XI$, $14 = XX$, $15 = XY$, $16 = YI$, $17 = YX$, $18 = YY$ with P signal acquisition.

1	2	6	12	13	1	2	6	12	14	1	2	9	12	16
1	2	9	12	17	1	3	5	11	13	1	3	5	11	15
1	3	8	11	16	1	3	8	11	18	1	5	6	11	13
1	5	6	12	13	1	5	11	13	16	1	5	11	13	17
1	6	12	13	16	1	6	12	13	18	1	8	9	11	16
1	8	9	12	16	1	8	11	13	16	1	8	11	14	16
1	9	12	13	16	1	9	12	15	16	2	3	4	10	14
2	3	4	10	15	2	3	7	10	17	2	3	7	10	18
2	4	6	10	14	2	4	6	12	14	2	4	10	14	16
2	4	10	14	17	2	6	12	14	17	2	6	12	14	18
2	7	9	10	17	2	7	9	12	17	2	7	10	13	17
2	7	10	14	17	2	9	12	14	17	2	9	12	15	17
3	4	5	10	15	3	4	5	11	15	3	4	10	15	16
3	4	10	15	18	3	5	11	15	17	3	5	11	15	18
3	7	8	10	18	3	7	8	11	18	3	7	10	13	18
3	7	10	15	18	3	8	11	14	18	3	8	11	15	18
4	5	9	15	16	4	5	9	15	17	4	6	8	14	16
4	6	8	14	18	4	8	9	14	16	4	8	9	15	16
4	8	10	14	16	4	8	11	14	16	4	9	10	15	16
4	9	12	15	16	5	6	7	13	17	5	6	7	13	18
5	7	9	13	17	5	7	9	15	17	5	7	10	13	17
5	7	11	13	17	5	9	11	15	17	5	9	12	15	17
6	7	8	13	18	6	7	8	14	18	6	7	10	13	18
6	7	12	13	18	6	8	11	14	18	6	8	12	14	18

read-outs for H and the II, IX, IY read-outs for P) instead of the complete 18 read-outs, the density matrix is

$$\rho_{12} = \begin{bmatrix} 0.37 & 0.31 - 0.13i & 0.29 + 0.034i & -0.074 - 0.17i \\ 0.31 + 0.13i & 0.28 & 0.37 + 0.0091i & -0.059 - 0.14i \\ 0.29 - 0.034i & 0.37 - 0.0091i & 0.25 & -0.058 - 0.17i \\ -0.074 + 0.17i & -0.059 + 0.14i & -0.058 + 0.17i & 0.094 \end{bmatrix}.$$

(15)

We see that the experimental density matrices are nearly identical for the two cases. Defining the error measurement

$$\delta = \left| \frac{\|\rho_{\text{exp}} - \rho_{\text{th}}\|_2}{\|\rho_{\text{exp}}\|_2} \right|,$$

(16)

where $\|\,\|$ is the norm of a matrix, we obtain the error of ρ_{all} relative to ρ_{th} 17%, and the same error of ρ_{12} to ρ_{th}, which roughly says that ρ_{all} or ρ_{12} is about 83% of ρ_{th}. Thus we have seen that the number of read-outs is reduced quite a lot, but the accuracy in the density matrix is not influenced much. For the extreme case with six read-outs only, the density matrix is

$$\rho_6 = \begin{bmatrix} 0.52 & 0.29 - 0.21i & 0.29 + 0.068i & -0.025 - 0.14i \\ 0.29 + 0.21i & 0.16 & 0.37 + 0.085i & -0.045 - 0.13i \\ 0.29 - 0.068i & 0.37 - 0.085i & 0.32 & 0.0039 - 0.15i \\ 0.025 + 0.14i & -0.045 + 0.13i & 0.0039 + 0.15i & 0.18 \end{bmatrix}.$$

(17)

Still, it is quite close to ρ_{th}. The relative error of ρ_6 to ρ_{th} is 32%. We see that, although the number of equations is reduced by more than half, the errors do not increase as much as one would think. Since the reconstruction of the density matrix in NMR quantum computing is so tedious, this work suggests a way of reducing the number of read-outs if the accuracy is not so highly required.

5. Summary

In conclusion, we have analysed the error matrix for the density matrix reconstruction in 2-qubit NMR quantum computing. We have found that the number of read-outs can be reduced greatly without significant loss in the accuracy. Our analysis can be easily extended to NMR systems with a larger number of qubits.

Acknowledgments

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