Analysis of Density Matrix reconstruction in NMR Quantum Computing

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Reconstruction of density matrices is important in NMR quantum computing. An analysis is made for a 2-qubit system by 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 density matrix reconstruction can be achieved even in a measurement with the number of read-outs being largely reduced.

I. INTRODUCTION

The study of quantum computers has attracted considerable attention since Shor in 1994 introduced a quantum mechanical algorithm for efficient factoring of large numbers\textsuperscript{1}. In another remarkable work, Grover in 1996 discovered that quantum mechanics can help to speed up data search in an unsorted database\textsuperscript{2}. 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.

How to realize quantum computing experimentally has sparked an explosion of interest. Among many proposed physical systems to implement quantum computation, such as trapped ions, optical photons, quantum dots, and so on, the NMR quantum computation is particularly attractive 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\textsuperscript{3,4} and a 5-qubit system\textsuperscript{5}, and for Grover’s algorithm with 2-qubit\textsuperscript{6} and 3-qubit systems\textsuperscript{7}. The order-finding problem in a 5-qubit system has recently been demonstrated in NMR\textsuperscript{8}, and a Cat state is prepared in a 7-qubit system\textsuperscript{9}.

The fundamental elements for information-processing in NMR are two-level nuclear spins that are bound together in a single molecule. Put forward in 1997 by Cory et al.\textsuperscript{10} and Gershenfeld et al.\textsuperscript{11}, the NMR scheme uses bulk numbers of molecules. The NMR technique 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 a 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 quantum state, or quantum state tomography, is not only important in quantum computation, but also important for general purposes. It has attracted many investigations. For instance, discrete Wigner function has been used to infer the quantum states of finite-dimensional systems from measurement by Leonhardt\textsuperscript{12,13}. Amiet and Weigert have studied various aspects of reconstruction of density matrix for a spin state in pure or mixed states\textsuperscript{14,15}. Reconstruction of state of light has been extensively studied by Leonhardt\textsuperscript{16}.

In NMR quantum computation, the liquid ensemble is described by the density matrix. The state of the NMR computer can be obtained by state tomography technique\textsuperscript{17}. 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 \textit{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 \textit{n} becomes moderately large.

In this paper, we study the reconstruction of density matrix in NMR. The mathematical structures of the density matrix reconstruction is analyzed. We found that the full state tomography read-outs, which consists 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 2-qubit density matrix in NMR experiment with the full read-outs and a much reduced read-outs respectively and found that they agree with the theoretical analysis.

The paper is arranged as follows. In Section II, we describe the procedures to construct the density matrix. We analyze the density matrix reconstruction procedure in section III. In Section IV, we discuss the reduction of 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 much reduced number of read-outs and at the same the loss of accuracy is small. Finally in Section V, we give a summary.

II. RECONSTRUCTION OF 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 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: \( II, IX, IY, XI, XX, XY, YI, YY, \) and \( YY \). Here, I, X and Y stand for, respectively, the identity operation, a 90 degree rotation about the x-axis, and a 90 degree rotation about the y-axis. Thus, in a state tomography, these operations are performed before NMR read-out measurements. We explain this through 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 separately carried out for H and P nuclear spins, and the nine operations are successively performed for each of them. This means that we have to perform totally \( 9 \times 2 = 18 \) read-outs.

Taking \( |↑⟩ = |1⟩ \) and \( |↓⟩ = |0⟩ \), the matrices of the nine operations are:

\[
\begin{align*}
II &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \\
IX &= \begin{bmatrix} 1/\sqrt{2} & -i/\sqrt{2} & 0 & 0 \\ -i/\sqrt{2} & 1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}, \\
XY &= \begin{bmatrix} 1/\sqrt{2} & 0 & i/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \\ -i/\sqrt{2} & 0 & 1/\sqrt{2} & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, \\
XX &= \begin{bmatrix} 1/\sqrt{2} & 0 & 0 & i/\sqrt{2} \\ 0 & 0 & 1 & 0 \\ 0 & -i/\sqrt{2} & 0 & 1/\sqrt{2} \\ -i/\sqrt{2} & 0 & 1/\sqrt{2} & 0 \end{bmatrix}.
\]

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

\[
\rho = \begin{bmatrix}
\rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\
\rho_{21}^* & \rho_{22} & \rho_{23} & \rho_{24} \\
\rho_{31}^* & \rho_{32}^* & \rho_{33} & \rho_{34} \\
\rho_{41}^* & \rho_{42}^* & \rho_{43} & \rho_{44}
\end{bmatrix} = \begin{bmatrix}
x_1 & x_2 + ix_{11} & x_3 + ix_{12} & x_4 + ix_{13} \\
x_2 - ix_{11} & x_5 & x_6 + ix_{14} & x_7 + ix_{15} \\
x_3 - ix_{12} & x_6 - ix_{14} & x_8 & x_9 + ix_{16} \\
x_4 - ix_{13} & x_7 - ix_{15} & x_9 - ix_{16} & x_{10}
\end{bmatrix}.
\]

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 \( \rho_{13} \) in Eq. (2) corresponds to the left peak of the spectrum of H, while the element \( \rho_{24} \) to the right peak of it. Similarly, the element \( \rho_{12} \) corresponds to the left peak of the spectrum of P, and the element \( \rho_{34} \) 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 labeled as 12, 13, 24 and 34 in the density matrix, and thus can be measured. The read-out gives the elements \( \rho'_{12}, \rho'_{13} \) and \( \rho'_{24}, \rho'_{34} \) 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 the size of \( 72 \times 16 \). 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, we have totally 73 equations. To determine the elements in the density matrix, one needs to solve the following set of linear equations for $x_i$:

$$\sum_{i=1}^{16} A_{\alpha i} x_i = B_\alpha, \quad \{\alpha = 1, 2, \ldots, 73\},$$  \tag{3}

where $A_{\alpha i}$ is the coefficient of $x_i$ in the $\alpha$-th equation and it varies with read-out for different rotations, and $B_\alpha$ 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 $\chi^2$ defined as

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

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

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

where

$$C_{ij} = \sum_{\alpha} A_{\alpha i} A_{\alpha j}, \quad \text{and} \quad b_i = \sum_{\alpha} B_\alpha A_{\alpha i}.$$  \tag{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 well determined in experiment. In the least square fitting procedure, these less well-determined matrix elements might possibly bring spurious values into the numerical calculation while leaving the $\chi^2$ value small. In other words, the $\chi^2$ might not be very sensitive in response to a big variation in experiment. For instance, if we have a set of equations, $x+y=e_1$, $x+1.001y=e_2$, this set of equations determines the sum of $x$ and $y$ very well, and the difference between $x$ and $y$ is poorly determined. The $\chi^2$ is insensitive to a change in $x-y$ while leaving $x+y$ unchanged.

III. AN ANALYSIS OF THE DENSITY MATRIX RECONSTRUCTION

In order to obtain the density matrix, one needs to use the least-square fitting method \cite{23} to derive them from the experimental data. Similar problem occurs actually 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. employed the error matrix method \cite{24} to analyze sensitivity of the nuclear structure to experimental input. In their method, instead of solving Eq. (3) directly, one first solves the eigenvalue problem for $C$ defined in (6),

$$UCU^+ = C_d.$$  \tag{7}

Here, $U$ is the unitary matrix that diagonalizes $C$. $C_d$ is called the error matrix \cite{24}. Then Eq. (3) becomes

$$C_{dy} = b',$$  \tag{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

$$y_i = \frac{b'_i}{(C_d)_{ii}}.$$  \tag{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 big 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 $y$'s 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

$$
C = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
$$

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 $y$’s are the combinations of the $x$ coefficients

$$
y_1 = -0.37x_3 + 0.82x_4 - 0.24x_6; \\
y_2 = -0.19x_1 + 0.41x_2 - 0.17x_3 - 0.32x_4 - 0.19x_5 - 0.59x_6 + 0.17x_7 - 0.19x_8 - 0.41x_9 - 0.19x_{10}; \\
y_3 = -0.0087x_1 - 0.093x_2 - 0.57x_3 - 0.39x_4 - 0.0087x_5 + 0.42x_6 + 0.57x_7 - 0.0087x_8 + 0.093x_9 - 0.0087x_{10}; \\
y_4 = 0.30x_1 - 0.30x_2 - 0.093x_3 - 0.26x_4 + 0.30x_5 - 0.61x_6 + 0.19x_7 - 0.30x_8 + 0.30x_9 + 0.30x_{10}; \\
y_5 = -0.35x_1 - 0.48x_2 + 0.027x_3 - 0.035x_4 - 0.35x_5 - 0.20x_6 - 0.027x_7 - 0.35x_8 + 0.48x_9 - 0.35x_{10}; \\
y_6 = -0.55x_2 + 0.44x_3 + 0.44x_7 - 0.55x_9; \\
y_7 = -0.44x_2 - 0.55x_3 - 0.55x_7 - 0.44x_9; \\
y_8 = 0.71x_5 - 0.71x_8; \\
y_9 = -0.71x_1 + 0.71x_{10}; \\
y_{10} = 0.50x_1 - 0.50x_5 - 0.50x_8 + 0.50x_{10}; \\
y_{11} = 0.71x_{12} + 0.71x_{15}; \\
y_{12} = -0.71x_{12} + 0.71x_{15}; \\
y_{13} = x_{13}; \\
y_{14} = x_{14}; \\
y_{15} = 0.71x_{11} - 0.71x_{16}; \\
y_{16} = 0.71x_{11} + 0.71x_{16}.
$$

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

IV. 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 the nine operations for $P$ and $H$, and plus 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 4 read-outs because there are altogether 16 unknowns. However, a detailed analysis of the rank of equations indicated that any 4 read-outs combined together can not provide sufficient numbers of independent equations. The minimum number of read-outs to be performed is
5. In table (I) we give the various set of 5 read-outs. In the table, operation 1 is the II with H signal acquisition (see table caption for details). From the table we see that not arbitrary combination of 5 operations are possible.

To see how well the density matrix is determined by a smaller number of read-outs, we choose a 6 read-outs 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:

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

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

$$
y_1 = -x_6; \quad y_2 = x_2; \quad y_3 = x_4; \quad y_4 = -0.79x_1 + 0.21x_5 + 0.58x_8; \quad y_5 = -0.21x_1 + 0.79x_5 - 0.58x_8; \quad y_6 = 0.71x_3 - 0.71x_7; \quad y_7 = 0.71x_3 + 0.71x_7; \quad y_8 = x_9; \quad y_9 = -0.50x_1 - 0.50x_5 - 0.50x_8 - 0.50x_{10}; \quad y_{10} = -0.29x_1 - 0.29x_5 - 0.29x_8 + 0.87x_{10}; \quad y_{11} = -0.71x_{12} + 0.71x_{15}; \quad y_{12} = 0.71x_{12} + 0.71x_{15}; \quad y_{13} = -0.71x_{13} - 0.71x_{14}; \quad y_{14} = -0.71x_{13} + 0.71x_{14}; \quad y_{15} = -0.71x_{11} - 0.71x_{16}; \quad y_{16} = -0.71x_{11} + 0.71x_{16}. \quad (12)
$$

The density matrix elements are as well determined as the one with 18 read-outs. However, the saving in the numbers of read-outs is great ($18 - 6 = 12$). Because we have less read-outs now, statistics in this case is surely poorer, and this will reduce 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 analyzed the density matrix for a 2-qubit system in an NMR experiment \[20\]. The theoretical prediction of the density matrix is

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

(13)
When constructing the density matrix using all 73 equations, we obtain

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

If we take only 49 equations out of the 73 equations, which means that we take only 12 read-outs (which contains all 9 read-outs for H and the II, IX, IY read-outs for P) instead of the complete 18 read-outs, the density matrix is

\[
\rho_{12} = \begin{bmatrix}
0.37 & 0.31 - 0.13i & 0.29 + 0.034i & -0.074 - 0.17i \\
0.31 + 0.13i & 0.28 & 0.37 + 0.009i & -0.059 - 0.14i \\
0.29 - 0.034i & 0.37 - 0.009i & 0.25 & -0.058 - 0.17i \\
-0.074 + 0.17i & -0.059 + 0.14i & -0.058 + 0.17i & 0.094
\end{bmatrix}.
\] (15)

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

\[
\delta = \frac{\|\rho_{\exp} - \rho_{1h}\|_2}{\|\rho_{\exp}\|_2},
\] (16)

where \(\|\cdot\|\) is the norm of a matrix, we get the error of \(\rho_{\text{all}}\) relative to \(\rho_{1h}\) 17\%, and the same error of \(\rho_{12}\) to \(\rho_{1h}\), which roughly says that \(\rho_{\text{all}}\) or \(\rho_{12}\) is about 83\% of \(\rho_{1h}\). Thus we have seen that the number of read-outs is reduced quite a lot, but the accuracy in the density matrix is not much influenced. For the extreme case with 6 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 \(\rho_{1h}\). The relative error of \(\rho_6\) to \(\rho_{1h}\) is 32\%. We see that, although the number of equations is reduced more than a 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, the present work suggests a way to reduce the number of read-outs if the accuracy is not so highly required.

V. SUMMARY

In conclusion, we have analyzed the error matrix for the density matrix reconstruction in the 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.

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

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