Determining the parity of a permutation using an experimental NMR qutrit

Shruti Dogra, Arvind and Kavita Dorai
Department of Physical Sciences, Indian Institute of Science Education & Research (IISER) Mohali, Sector 81 SAS Nagar, Manauli PO 140306 Punjab India.

We present the NMR implementation of a recently proposed quantum algorithm to find the parity of a permutation. In the usual qubit model of quantum computation, speedup requires the presence of entanglement and thus cannot be achieved by a single qubit. On the other hand, a qutrit is qualitatively more quantum than a qubit because of the existence of quantum contextuality and a single qutrit can be used for computing. We use the deuterium nucleus oriented in a liquid crystal as the experimental qutrit. This is the first experimental exploitation of a single qutrit to carry out a computational task.

I. INTRODUCTION

Quantum information processors exploit intrinsic quantumness of quantum systems to perform computational tasks more efficiently than their classical counterparts [1, 2]. The notion of quantumness of a quantum system has many aspects, including quantum entanglement [3, 4], contextuality [5–8], nonlocality [9] and fragility toward quantum measurements [10]. A qubit is the building block of a standard quantum computer, however a single qubit does not possess intrinsic quantum features. In fact, the polarization states of a classical beam of light provide a classical system with exactly the same properties as that of a single qubit. Therefore, by manipulating the polarization states of a classical beam of light via half-wave and quarter-wave plates, one can efficiently simulate a single qubit [11, 12]. In a quantum computer, we invariably have multiple qubits and can create highly entangled states of these qubits which are exploited to perform computation [13, 14]. There is no classical physical system on which we can generate such entangled states because the concept of multi-qubit entanglement is an intrinsically quantum phenomenon. Therefore, although a single qubit cannot be used to do any effective quantum computation, multiple qubits can in fact provide a computational resource. Scaling issues in algorithmic implementations of the and achieving computational speedup without entanglement has been discussed in [15, 17]. On the contrary, a single qutrit (a three-level quantum system) has no classical counterpart [18]. It is the simplest quantum system where the notion of contextuality can be introduced [19]. Quantum contextuality is a strange property of quantum systems where measurement outcomes of an observable A depend on the “context” in which we perform the measurement, the context being the set of other observables which are measured along with A (that commute with A and among themselves). For a qutrit, for a given observable, we can have more than one context, and therefore a qutrit possesses contextuality. In contrast, for a qubit, for every observable there is only one context. This makes a case for considering a single qutrit as a possible resource for quantum computation. A recent paper explores this possibility in a concrete context of determining the parity of a given permutation of three objects [20]. They have shown in their model algorithm that for the six possible permutations (three even and three odd), the parity can be determined by a single call to the quantum oracle, as opposed to two calls in the classical setup. The algorithm can be generalized to higher-dimensional qudits with the same two to one speedup ratio. This work is an interesting development because it uses the quantumness of a single system, where there is no question of entanglement, to perform a computation. The author also alludes to the possibility of the contextuality of a qutrit playing a role in this speedup. Recent work on quantum information processing with qutrits includes the description of unitary gates [21], a quantum circuit to solve systems of linear equations [22], a fundamental test of nonclassicality [23, 24], the measurement of entangled qudits [25], experimental quantum cryptography [26], to study entanglement sudden death [27], and an experimental test of quantum contextuality [28].

In this work we implement the parity determining quantum algorithm on an NMR quantum information processor. Recent work on qudit computation using NMR includes a study of relaxation dynamics in a quadrupolar system [29], the preparation of pseudopure states in a single qutrit [30], the emulation of a qudit-qubit system using strongly dipolar coupled spin-1/2 particles [31], and state tomography and logical operations in a three qubits NMR quadrupolar system [32]. Here we have used a deuterium (spin-1 particle) nucleus as the NMR qutrit. When a strong magnetic field is applied, the three levels of the spin-1 deuterium nucleus Zeeman split and provide us with two degenerate transitions. The degeneracy is lifted by orienting the system in a liquid crystal matrix where the anisotropic environment leads to a contribution of the dipolar coupling to the Hamiltonian. To the best of our knowledge, this is the first experimental exploitation of the quantumness of a single qutrit for quantum computation.

The material in this paper is arranged as follows: Sec-

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*shrutidogra@iisermohali.ac.in
arvind@iisermohali.ac.in
lavita@iisermohali.ac.in
tion [11] describes the parity determination quantum algorithm given in [20]. Section [11] contains a description of the quantum circuit constructed to experimentally implement the parity algorithm, details of the experimental NMR qutrit, and a discussion of the results. Section [IV] contains some concluding remarks.

II. PARITY DETERMINING ALGORITHM

A qutrit-based black-box algorithm has been recently designed to evaluate the parity of permutation of three objects by one oracle call, whilst the classical algorithm requires two oracle calls [20]. Since the algorithm uses a single qutrit and has a quantum advantage, the authors conjecture that this computational speedup may be attributed to contextuality, an intrinsic quantum feature present in a qutrit.

Consider the six possible permutations of the three objects in the set \{1, 2, 3\}, categorized as even or odd, depending on whether the number of exchange operations performed is even or odd. The computational task that one wants to perform is to find the parity of the permutation. If we consider the permutation as a function \( f(x) \) where \( x \in \{1, 2, 3\} \), then to determine the parity classically we need to evaluate \( f(x) \) for at least two values of \( x \).

In the quantum setting, let us consider a qutrit with its eigen states labeled by its spin quantum number \( |m\rangle \) where \( m = 1, 0, -1 \). The action of permutations on these states are the bijective maps \( f : \{1, 0, -1\} \rightarrow \{1, 0, -1\} \). The six possible maps can be written down using Cauchy’s notation. The three even maps and the corresponding unitary transformations are given by:

\[
\begin{align*}
\mathbf{U}_1 & = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
\mathbf{U}_2 & = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 1 \\ 0 & -1 & 1 \end{pmatrix} \\
\mathbf{U}_3 & = \begin{pmatrix} 1 & 0 & -1 \\ 1 & 1 & 0 \\ 0 & 1 & 0 \end{pmatrix}
\end{align*}
\]

while the three odd maps and the corresponding unitary transformations are given by:

\[
\begin{align*}
\mathbf{U}_4 & = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \end{pmatrix} \\
\mathbf{U}_5 & = \begin{pmatrix} 1 & 0 & -1 \\ 1 & -1 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\
\mathbf{U}_6 & = \begin{pmatrix} 1 & 0 & -1 \\ 1 & 0 & -1 \\ 0 & -1 & 1 \end{pmatrix}
\end{align*}
\]

The quantum oracle thus is a black box which performs the unitary transformation corresponding to a given permutation on the input state of the qutrit.

A direct run of the oracle on the eigen states of the qutrit obviously does not help, and we would still require two oracle calls, as in the classical case. The quantum algorithm thus begins by preparing a superposition of eigen states by the action of the quantum Fourier transformation for a qutrit acting on an initial state (we consider the state \( |\pm 1\rangle \)) and defined through the unitary operation

\[
F = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & e^{2\pi i/3} & e^{4\pi i/3} \\ 1 & e^{-2\pi i/3} & e^{2\pi i} \end{pmatrix}
\] (3)

This is followed by the oracle call which is a black box operation where the unitary operator \( U_f \) (corresponding to the function \( f_k \)) is applied to the superposition state created by the quantum Fourier transformation. The output state is then subjected to an inverse Fourier transformation which brings the state back to one of the eigen states of the qutrit up to a phase factor. The final state of the qutrit is either \( |\pm 1\rangle \) (if \( f_k \) is even) or \( |0\rangle \) (if \( f_k \) is odd). The final state for the case of even functions is orthogonal to the final state for the case of odd function and are thus distinguishable by a measurement on a single copy. The result of such a measurement in the \( \{|1\rangle, |0\rangle, |\pm 1\rangle \} \) basis will thus reveal the parity of the corresponding permutation.

![Quantum circuit to determine the parity of the permutation of three objects in a single step. The initial state is the pure state of a single qutrit, \( |\pm 1\rangle \). Fourier transformation and its inverse are represented as \( ‘F’ \) and \( ‘F^{-1}’ \). The black box carrying out the permutations has six different possibilities. ‘I’ is the identity operator, while ‘S12’, ‘S23’ and ‘S13’ are SWAP operators describing a swap between levels 1 – 2, 2 – 3 and 1 – 3 of a single qutrit respectively.](image)

The unitaries corresponding to different functions can be constructed using combinations of SWAP operators as...
shown in Figure 1. The even unitaries are constructed by the identity operator (no operation), and by two sequential non-commuting swap gates $S_{12}$ and $S_{23}$, where the $S_{ij}$ gate performs a swap between the $i$th and $j$th levels. The odd unitaries are constructed by the single swap $S_{12}, S_{23}$ and $S_{13}$ respectively.

III. NMR IMPLEMENTATION OF THE PARITY ALGORITHM

A. The NMR Qutrit

![Diagram of the NMR qutrit](image)

**FIG. 2.** A single NMR qutrit is constructed by orienting deuterated Chloroform in a lyotropic liquid crystal, with the deuterium, (spin 1) being the single qutrit: (a) the Chloroform-D molecule, (b) the energy level diagram of a single qutrit. Energy levels are numbered as 1, 2, and 3 and the corresponding basis vectors are represented on the right. Relative populations of the energy levels at equilibrium are shown with red circles. Two spectral lines in an NMR spectrum of a single qutrit result from the transitions between energy levels 1-2 and 2-3 as shown with arrows. (c) The deuterium NMR spectrum of Chloroform-D with the transitions labeled as Line 1 and Line 2. The experiments were performed at 277 K resulting in a quadrupolar splitting of 936 Hz.

We use the deuterated chloroform molecule oriented in a lyotropic liquid crystal as our system, where the deuterium nucleus serves as the single qutrit. The lyotropic liquid crystal is composed of 25.6\% of Potassium Laurate, 68.16\% of $H_2O$ and 6.24\% of Decanol, and 50 µl of Chloroform-D is added to 500 µl of liquid crystal.

The deuterium NMR spectrum of oriented Chloroform-D was acquired at different temperatures, as this system possesses a liquid crystalline phase for a wide range of temperature. Figure 2 shows the energy level diagram of the three level system along with the relative populations in the presence of a strong magnetic field $B_0$. The energy levels are numbered as $\{|+1\rangle, |0\rangle, |-1\rangle\}$ respectively, and the single quantum transitions are labeled with arrows. Figure 2(c) shows the deuterium NMR spectrum of oriented Chloroform-D; the spectral lines corresponding to transitions 1-2 and 2-3 are labeled as Line 1 and Line 2 respectively.

For a deuterium nucleus with spin $I = 1$, the electric quadrupole moment of the nucleus interacts with the electric field gradients generated by the surrounding electron cloud, leading to a quadrupolar coupling term in the Hamiltonian

$$H = -\omega_0 I_z + \frac{eQV_{zz}}{4I(2I-1)} (3I_z^2 - I^2)$$

where the first term describes the Zeeman interaction and the second term describes the first-order quadrupolar interaction, $Q$ is the quadrupolar moment and $V_{zz}$ is the average value of the uniaxial electric field gradient component over the molecular motion.

In an isotropic environment the electric field gradient component $V_{zz}$ averages to zero, and the quadrupolar term in the Hamiltonian vanishes. The two single-quantum transitions become degenerate and thus cannot be distinguished. For quantum computing and gate implementation on the deuterium qutrit, one requires the two single-quantum transitions to be separately manipulatable, which is not possible with liquid-state NMR methods. To resolve this problem, the molecule is embedded in a liquid crystalline environment and the anisotropic molecular orientation with respect to the strong magnetic field, gives rise to a finite quadrupolar coupling term in the Hamiltonian now given by

$$H = -\omega_0 I_z + \Lambda (3I_z^2 - I^2)$$

where $\Lambda = \frac{e^2qQS}{4}$ is the effective value of the quadrupolar coupling, $eq = V_{zz}$ denotes the field gradient parameter, and $S$ is the order parameter of the liquid crystal. This effective quadrupolar coupling term is responsible for the splitting between the previously degenerate energy levels and hence for the two non-degenerate lines in the NMR spectrum. This term could be very large (in MHz) but its contribution is tunable by the order parameter $S$ of the liquid crystal, and a small value of $S$ reduces the effective quadrupolar coupling to a few hundred Hz. At 277 K, the effective quadrupolar splitting between the spectral lines was measured to be 936 Hz, and all the experiments were performed at this temperature.
B. Experimental Results

FIG. 3. (a) Pulse sequence for the implementation of the parity algorithm on a single qutrit. The first two channels of the pulse sequence correspond to the two NMR transitions. The first 90° pulse on Line 1 followed by a gradient g1 creates the pseudopure state |−1⟩. The next three pulses perform the Fourier transformation. (b) The black box carries out the six possible permutations corresponding to the three even and three odd functions. The two channels inside the black box correspond to the two NMR transitions of a single qutrit. A 30° non-selective detection pulse preceded by a clean up gradient g2 is applied to evaluate the final result of the computation. All the 90° pulses are shown in blue, 270° in red and 180° in black. Non-selective pulses are shown as a common rectangle for both the transitions. Pulse angles and the axes of rotations are shown corresponding to each pulse. All the pulses are shaped pulses. (270)−x23 (109.47)−y12 (90)−y23. This leads to the superposition state $\frac{1}{\sqrt{3}}(|+1⟩+e^{\frac{2\pi i}{3}}|0⟩+e^{\frac{-2\pi i}{3}}|−1⟩)$. When this state undergoes odd permutations we obtain the states $\frac{1}{\sqrt{3}}(e^{-2\pi i/3}|+1⟩+|0⟩+e^{2\pi i/3}|−1⟩)$, $\frac{1}{\sqrt{3}}(|+1⟩+e^{2\pi i/3}|0⟩+ e^{-2\pi i/3}|−1⟩)$ and $\frac{1}{\sqrt{3}}(e^{2\pi i/3}|+1⟩+e^{-2\pi i/3}|0⟩ + |−1⟩)$ respectively. Inverse Fourier transform of these states result in the states $e^{-2\pi i/3}|0⟩$, $|0⟩$ and $e^{2\pi i/3}|0⟩$ respectively. For even permutations, the initial state is unchanged, up to a global phase. The permutations are implemented by various combinations of 180° transition-selective as well as non-selective pulses as detailed in Figure 3(b). The non-selective pulses act on both the transitions and are shown as a common rectangle on both the lines. The final state is detected by a 30° non-selective detection pulse preceded by a clean up gradient g2. All the transition-selective pulses used in this work are 4 ms long ‘Gaussian’ shaped pulses and the non-selective ones are ‘Sinc’ shaped pulses with a duration of 0.5 ms. There is no gradient implementation while permuting the elements. The entire set of pulses used to perform the algorithm were implemented before decoherence sets in.

The deuterium NMR spectrum obtained after the six different permutations is shown in Figure 4. There are two possible resultant states after the computation is performed, depending upon whether the permutation is even or odd. If the permutation is even, the final state is $e^{\phi}|−1⟩$ and if it is odd, the final state is $e^{\phi}|0⟩$. These two final states are orthogonal to each other and can hence be distinguished by a single projective measurement. Since projective measurements are not possible on an ensemble NMR quantum computer, we use their spectral signature to distinguish these two orthogonal states. The state |−1⟩, when detected by applying a 30° non-selective pulse on both the transitions, gives rise to a line corresponding to transition 2-3 and the state |0⟩ with the same detection pulse gives two lines at transitions 1-2 and 2-3 with equal and opposite intensities. Global phases are not detectable in NMR experiments and can hence be ignored.

Figure 4 depicts the phase corrected spectra (at the same intensity scale) corresponding to six different permutations. The spectra on the left correspond to the final state |−1⟩ after an even permutation, while the spectra on the right correspond to the final state |0⟩ after an odd permutation.

IV. CONCLUDING REMARKS

We have experimentally implemented a parity determining algorithm on a single NMR qutrit, which does not require entanglement to achieve computational speedup. We have oriented the deuterium qutrit in a liquid crystalline environment bringing in a difference in the resonance frequencies of the two transitions, which was a key component in allowing us to manipulate the qutrit states. Although the demonstration of the computing
Even Odd

(1) (4)

(2) (5)

(3) (6)

Even Odd

$\omega_D$ (in ppm) $\omega_D$ (in ppm)

FIG. 4. The NMR spectra after implementing the parity determining algorithm on a single qutrit. Spectra (numbered 1 to 6) correspond to the six possible permutations. All the spectra were obtained by applying a $30^\circ$ non-selective detection pulse on both the transitions. Spectra 1,2,3 correspond to the state $|\text{ }^{-1}\rangle$ (resulting from an even permutation) and spectra 4,5,6 correspond to state $|\text{ }0\rangle$ (resulting from an odd permutation).

Acknowledgments All experiments were performed on the Bruker 600 MHz FT-NMR spectrometer in the NMR Research Facility at IISER Mohali. SD was funded by a Government of India UGC-SRF fellowship.

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