NMR investigation of contextuality in a quantum harmonic oscillator via pseudospin mapping

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received 5 November 2015; accepted in final form 28 January 2016
published online 16 February 2016

PACS 03.65.Ta – Foundations of quantum mechanics; measurement theory
PACS 03.67.-a – Quantum information
PACS 03.65.Ud – Entanglement and quantum nonlocality (e.g. EPR paradox, Bell’s inequalities, GHZ states, etc.)

Abstract – Physical potentials are routinely approximated to harmonic potentials. Hence it is important to know when a quantum harmonic oscillator (QHO) behaves quantum mechanically and when classically. Recently Su et al. (Phys. Rev. A, 85 (2012) 052126) have theoretically shown that QHO exhibits quantum contextuality (QC) for a certain set of pseudospin observables. Here we encode the four eigenstates of a QHO onto four Zeeman product states of a pair of spin-(1/2) nuclei. Using the techniques of NMR quantum information processing, we then demonstrate the violation of both state-dependent and state-independent inequalities arising from the noncontextual hidden variable model.

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Introduction. – Quantum contextuality (QC) states that the outcome of the measurement depends not only on the system and the observable but also on the context of the measurement, i.e., on other compatible observables which are measured along with [1-4].

Let us consider a pair of space-like separated entangled particles, with local observables A and C belonging to the first particle, and B and D to the second. We assume that these observables are dichotomic (i.e., can take values ±1) and that the pairs (A, B), (B, C), (C, D), and (D, A) commute.

Classically, one assigns objective properties to the particles such that D behaves identically on the state of the system irrespective of whether it is measured in the context of A or in the context of C, even though A and C are not compatible [5,6]. Such measurements are said to be context independent. Classically, one can pre-assign values (a, c) to (A, C) of the first particle independent of the measurement carried out on the second particle. Similarly, for the second particle one can pre-assign values (b, d) to (B, D) independent of the measurement carried out on the first particle. In these pre-assignments, implicit is the assumption of noncontextual hidden variables, which predict definite measurement outcomes independent of the measuring arrangement. If we pre-assign values to observables such that A, B, C, D = ±1, it follows that

\[ I = \langle AB + BC + CD - AD \rangle = \langle AB \rangle + \langle BC \rangle + \langle CD \rangle - \langle AD \rangle \leq 2 \]  

(see ref. [7]). This inequality often known as Clauser-Horne-Shimony-Holt (CHSH) inequality arises from the noncontextual hidden variable (NCHV) model and must be satisfied by all classical particles.

Now let us see the implication of the quantum theory. Let Alice and Bob share a large number of singlet states: \((|01\rangle - |10\rangle)/\sqrt{2} = -(|+\rangle - |-\rangle)/\sqrt{2}\), where \(|0\rangle\) and \(|1\rangle\) are eigenstates of Pauli z-operator \((\sigma_z)\) and \(|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}\). Alice measures on her qubit either \(\sigma_z^A\) or \(\sigma_x^A\), while Bob always measures \(\sigma_z^B\). Let us compare the results of only those measurements in which Alice has obtained the outcome +1. If Alice measures \(\sigma_z^A\), then Bob’s qubit collapses to \(|1\rangle\) = \((|+\rangle - |-\rangle)/\sqrt{2}\). In this context (i.e., \(\sigma_z^A\)), Bob will get both outcomes ±1 with equal probability. On the other hand, if Alice measures \(\sigma_x^A\) on her qubit, then Bob’s qubit collapses to \(|-\rangle\) and, in this context (i.e., \(\sigma_x^A\)), Bob will always get the outcome −1. Hence the context dependence.

Here we experimentally investigate QC of a quantum harmonic oscillator (QHO). There is a variety of quantum

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systems whose potentials are approximated by QHO. Consider, for example, the quantized electromagnetic field used to manipulate a qubit in cavity quantum electrodynamics [8]. Recently, QC in QHO has been theoretically studied by Su et al. [9] by mapping four lowermost QHO states onto four pseudospin states. Such states can be encoded by qubit states, and QC can be studied by realizing the measurements of appropriate observables. In this work, we realize this study using a nuclear magnetic resonance (NMR) quantum simulator [10].

In the following section we shall revisit the formulation of Su et al., and in the third section, we describe the experimental demonstration of state-dependent and state-independent QC using an NMR system. Finally we present our conclusions in the last section.

**Theory.** – Su et al. [9] have theoretically studied QC of eigenstates of a one-dimensional quantum harmonic oscillator (1D-QHO) by introducing two sets of pseudospin operators,

\[ \Gamma = (\Gamma_x, \Gamma_y, \Gamma_z), \quad \Gamma' = (\Gamma'_x, \Gamma'_y, \Gamma'_z) \]

with components

\[ \Gamma_x = \sigma_x \otimes I, \quad \Gamma_y = \sigma_y \otimes \sigma_y, \quad \Gamma_z = -\sigma_y \otimes \sigma_y, \]

\[ \Gamma'_x = \sigma_x \otimes \sigma_x, \quad \Gamma'_y = I \otimes \sigma_y, \quad \Gamma'_z = -\sigma_x \otimes \sigma_x, \quad (2) \]

where \( I \) is 2 \times 2 identity matrix. Using these operators they defined the following unitary observables:

\[ \begin{align*}
A &= \Gamma_x = \sigma_x \otimes I, \\
B &= \Gamma'_x \cos \beta + \Gamma'_y \sin \beta = \sigma_x \otimes (\sigma_z \cos \beta - \sigma_x \sin \beta), \\
C &= \Gamma_z = -\sigma_y \otimes \sigma_y, \\
D &= \Gamma'_x \cos \eta + \Gamma'_y \sin \eta = \sigma_x \otimes (\sigma_z \cos \eta - \sigma_x \sin \eta). \quad (3)
\end{align*} \]

The products which form the inequality expression (1) are

\[ \begin{align*}
AB &= I \otimes (\cos \beta \sigma_z - \sin \beta \sigma_x), \\
BC &= -\sigma_x \otimes (\cos \beta \sigma_z + \sin \beta \sigma_x), \\
CD &= -\sigma_z \otimes (\cos \eta \sigma_x + \sin \eta \sigma_z), \\
DA &= I \otimes (\cos \eta \sigma_x - \sin \eta \sigma_z). \quad (4)
\end{align*} \]

Here the following commutation relations hold: \([I_i, I_j] = 0 \) \((i,j = x,y,z)\), \([\Gamma_x, \Gamma_y] = 2i\Gamma_z\), \([\Gamma'_x, \Gamma'_y] = 2i\Gamma'_z\), and similar relations with cyclic permutations of \(x,y,z\). The observables \(A,B,C,D\) have eigenvalues \(\pm 1\), with \((A,B), (B,C), (C,D), \text{ and } (D,A)\) forming compatible pairs.

Su et al. [9] have shown that

\[ \Gamma'_{QHO}^{QM} = 2\sqrt{2} > 2, \quad \text{when } (\beta, \eta)_l = \begin{pmatrix} (-\pi/4, -3\pi/4)_0, \\ (3\pi/4, \pi/4)_1, \\ (\pi/4, 3\pi/4)_2, \\ (-3\pi/4, -\pi/4)_3, \end{pmatrix} \quad (5) \]

where \( \Gamma'_{QHO}^{QM} \) is the expression on l.h.s of inequality (1) for \( l = 0, 1, 2, \text{ and } 3\), and \( |0\>_{QHO}, |1\>_{QHO}, |2\>_{QHO}, \text{ and } |3\>_{QHO} \) of the first four energy eigenstates of 1D-QHO. Thus, QHO violates the inequality (1) for certain observables and thereby exhibits QC.

It is well known that only certain two-particle states violate the CHSH inequality (1). As shown in [11,12] factorable states always satisfy inequality (1) for local observables, which are of the form \( P \otimes I \) or \( I \otimes Q \) [13]. With maximally mixed state \(|\mathbb{I}/2 \otimes \mathbb{I}/2\rangle\rangle\) the inequality (1) is satisfied even with nonlocal observables in eq. (3), which are of the form \( P \otimes Q \) measured nonlocally/jointly [13], which is obvious from the fact that all the products in eq. (4) are traceless. However, if the initial state is nonfactorable, we can always find observables such that inequality (1) is violated [11]. Although the pseudospin states \(|00\>, |01\>, |10\>, |11\>\rangle\rangle\) are factorable, they still violate (1) since the observables in eq. (3) are nonlocal. Thus, we observe that even when a system is in a nonentangled state, measurements of nonlocal observables may lead to violation of noncontextuality inequality [14].

**State-independent QC:** There exist stronger inequalities obtained from NCHV models which are violated by all states, including separable or maximally mixed states. If the initial state is maximally mixed, entanglement cannot be created by measuring whatever observable (local or nonlocal). This shows that entanglement is not necessary in general even in a bipartite system, to exhibit QC. In this sense, it can be argued that QC is more fundamental or general than entanglement. Any system whose Hilbert space has dimension \( \geq 2 \) exhibits QC [4]. Even a single spin-1 particle (where entanglement has no meaning as far as the spin degree of freedom is concerned) can exhibit QC [15].

**Experiment.**

**State-dependent contextuality.** To experimentally study the inequality (1), we need to realize the following processes:

i) To physically map various energy eigenstates of 1D-QHO: We encode the first four energy eigenstates \{|0\>_{QHO}, |1\>_{QHO}, |2\>_{QHO}, |3\>_{QHO} \} onto the four Zeeman energy eigenstates \{|00\>, |01\>, |10\>, |11\>\rangle\rangle\} of a pair of spin-(1/2) nuclei (i.e., two qubits) precessing in external static magnetic field. In fact any four arbitrarily chosen energy eigenstates of 1D-QHO and also their superposition states exhibit QC [9].

ii) To extract the joint expectation values for operators \( AB, BC, CD \), and \( DA \). The Moussa circuit shown in fig. 1 [16,17], is used to extract the expectation values of observables in a joint measurement. Since this protocol needs an ancillary qubit, in all we need to have three qubits with sufficiently long coherence times.

The three qubits for this experiment were provided by the three \(^{19}\text{F}\) nuclear spins of trifluoroiodoethylene.
In our experiments, all the controlled operations were realized by numerically optimized radio frequency (RF) pulses obtained using the GRAPE technique [20]. Each pair of controlled operations in circuit 1 was realized by a GRAPE sequence with a duration of about 23 ms (having RF segments of duration 5 μs) and an average Hilbert-Schmidt fidelity better than 0.99 over a 10% variation in the RF amplitude.

We estimated the values for $I_1$ (1), for all the four eigenstates and independently varied both $\beta$ and $\eta$ over the range $[-\pi, \pi]$ with increments of $\pi/4$. The results are shown in fig. 3. The maximum experimental values for $I_0$, $I_1$, $I_2$, and $I_3$ are $2.40 \pm 0.02$, $2.45 \pm 0.02$, $2.39 \pm 0.02$, and $2.42 \pm 0.03$, respectively. These values being greater than 2 clearly violate the classical bounds and hence prove QC of QHO. However, values lower than the maximum theoretical violation (i.e., $2\sqrt{2} = 2.82$) are presumably due to the decoherence intrinsic to the quantum system and other experimental imperfections.

State-independent contextuality. Su et al. have also studied the state-independent contextuality [9,21] by considering the inequality (arising from the NCHV model)

$$
\langle P_{11}P_{12}P_{13} \rangle + \langle P_{21}P_{22}P_{23} \rangle + \langle P_{31}P_{32}P_{33} \rangle + \langle P_{11}P_{21}P_{31} \rangle + \langle P_{12}P_{22}P_{32} \rangle - \langle P_{13}P_{23}P_{33} \rangle \leq 4, \tag{9}
$$

where $P_{ij}$ are the elements of the matrix $P$.

$$
P = \begin{pmatrix}
\Gamma_z & \Gamma'_z & \Gamma_z\Gamma'_z \\
\Gamma'_z & \Gamma_x & \Gamma_x\Gamma'_z \\
\Gamma_z\Gamma'_z & \Gamma_x\Gamma'_z & \Gamma_y\Gamma'_y
\end{pmatrix} \tag{10}
$$

Fig. 1: (Colour online) Moussa protocol for extracting the expectation value of the joint observable $X_1X_2X_3$, i.e. $(X_1X_2X_3)$. Here $X_i$s are mutually commuting unitary observables.

Fig. 2: (Colour online) (a) Molecular structure, (b) resonance off-sets (diagonal elements) and $J$-couplings (off-diagonal elements) in Hz of trifluoriodoethylene, and (c) pulse sequence for pseudopure state preparation. In (c), 180° pulses are represented by unshaded rectangles, and other pulses by shaded rectangles with tilt angles and phases as indicated. The lowest row consists of pulsed field gradients (PFG) used to destroy the transverse magnetization.
Here, in each row (column) of the matrix $P$, every observable commutes with every other. $P_{ij}$ are dichotomic observables with measurement outcomes $\pm 1$. We can verify the inequality (9) by pre-assigning the values $\pm 1$ to each observable $P_{ij}$.

Now introducing the operators from expressions (2), we find that the product of each row of the matrix $P$ is an identity (i.e., $P_{ij}P_{jk}P_{kl} = 1$). Similarly, the products along each of the first two columns again become an identity. However, the product along the last column can satisfy the condition that the product along each row and along the first two columns be $+1$ and along the last column be $-1$. This shows that the quantum theory is not compatible with the NCHV model.

Further, the expectation values for the first five operators in expression (9) are all $+1$ while that of the last term is $-1$. Therefore, for an arbitrary state, the quantum upper bound for the lhs of expression (9) is 6, while the classical upper bound is 4 [9].

To investigate state-independent QC, we need to measure the joint expectation values of three observables. We again use the circuit 1 for this purpose. Taking advantage of the state-independent property of the above-mentioned inequality, we choose the thermal equilibrium state (6) as initial state. A $(\pi/2)_{y}$ pulse was applied on the first spin to prepare the ancilla in a superposition state. Then state (6) takes the form $(1 - 4\epsilon)I_{8}/8 + \epsilon(|+\rangle\langle+| \otimes I \otimes I) + \epsilon(I_{2} + I_{3})$.

All the controlled $P_{ij}$ operations were realized using the GRAPE sequences having average fidelities better than 0.99 over 10% variation in RF amplitude. The total duration of the RF sequences for each term in inequality (9) were about 40 ms. The experimentally obtained value of the lhs of inequality (9) is $4.81 \pm 0.02$. Thus, we observed a clear violation of the classical bound. However, it is still lower than 6, the quantum limit. The reduced violation can again be attributed to decoherence and other experimental imperfections.

**Conclusions.** We have experimentally demonstrated the quantum contextuality exhibited by first four energy eigenstates of a 1D-QHO by mapping them to a Zeeman energy eigenstates of a pair of NMR qubits. The continuous observables of the harmonic oscillator are then mapped onto certain pseudospin observables measured on the qubits. We have used the Moussa protocol to retrieve the joint expectation values of the observables using an ancillary qubit. Thus, our quantum register was based on three mutually interacting spin-(1/2) nuclei controlled by NMR techniques. The experimental results clearly violate the classical bound proving contextuality in the quantum harmonic oscillator.

We also studied a state-independent quantum contex-
tuality by measuring a set of expectation values on the thermal equilibrium states of the nuclear spins. Exper-
iments again revealed a clear violation of the classical bound. These results not only establish the validity of quantum theoretical calculations, but also highlight the success of NMR systems as quantum simulators.

### Acknowledgments

Authors are grateful to Prof. Dipankar Home for referring us to Hong-Yi Su et al.’s paper [9] and also for his valuable suggestions and discussions. We also thank Siddharth Das and Abhishek Shukla for useful discussions. This work was partly supported by DST Project No. SR/S2/LOP-0017/2009.
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