Experimentally simulating the violation of Bell-type inequalities for three qubits by NMR

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We simulate the violation of MABK inequality for a three-qubit GHZ state in a NMR system. Furthermore, for generalized GHZ states, we test two different Bell's inequalities, i.e., MABK inequality and Chen's inequality. The experimental results show that Chen's inequality is more efficient than MABK inequality for any generalized GHZ entangled states.

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I. Introduction

In 1964, Bell showed that in all local realistic theories, correlations between the outcomes of measurements in different parts of a physical system satisfy a certain class of inequalities [1]. However, it was easy to find that entangled states violate these inequalities in quantum mechanics, which shows the crucial conflict between classical theory and quantum mechanics. Hence, Bell's work was described as "the most profound discovery of science" [2] or "one of the greatest discoveries of modern science" [3]. Later, many important generalizations, including the Clauser-Horne-Shimony-Holt (CHSH) [4] and Mermin-Ardehali-Belinskii-Klyshko (MABK) inequalities [5] have been developed. More recently, Werner and Wolf and Żukowski and Brukner (WWZB) derived a set of multipartite Bell inequalities, by using two dichotomic observables per site [6]. There has been increasing interest in the subject of Bell's inequalities, because of not only fundamental problems of quantum mechanics, but also their relation to quantum communication [7, 8, 9] and quantum cryptography [10, 11]. For example, the security of some quantum communication protocols are based on the loophole-free violation of Bell inequalities [11, 12, 13]. Furthermore, Bells inequalities can be a useful tool to detect entanglement which is a powerful computational resource in quantum computation [14].

Various experiments to test Bell inequality have been performed in a wide range of systems including photons [15, 16, 17], atoms systems [18, 19, 20], atomic ensembles [21, 22], and trapped ions [23]. Recently, an experiment to simulate the violation of CHSH inequality has been carried out in an NMR system [24]. These experiments were mainly carried out on the maximal entangled states, such as Bell states and standard GHZ states, etc, rarely on nonmaximal entangled states, such as generalized GHZ states. However, many phenomena can be disclosed by nonmaximal entangled states, for instance, the nonmaximal entangled states make the maximal violation of many Bell-type inequalities [26, 27]. There are still many open problems about the Bell-type inequalities with nonmaximal entangled states. Therefore, it is interesting and meaningful to study the case of nonmaximal entangled states.

For three-qubit generalized GHZ states

$$|\Psi\rangle = \cos\theta\,|000\rangle + \sin\theta\,|111\rangle\,, \tag{1}$$

which $\theta \in [0, \frac{\pi}{2}]$, Scarani and Gisin [30] firstly found that there exist a region of them satisfying the MABK inequality. It is shown that for $\theta \leq \pi/12$ or $\theta \geq 5\pi/12$ the states (1) do not violate the three-qubit MABK inequality. Later on, Żukowski *et.al* proved that [34] (i) for $N = even$, the generalized GHZ states violates the WWZB inequality, rather than MABK inequalities; (ii) for $N = odd$ and $sin(2\theta) \leq 1/\sqrt{2^{N-1}}$, (the correlations between measurements on qubits in the generalized GHZ state satisfy all Bell inequalities for correlation functions, which involve two dichotomic observables per local measurement station ???). Chen and Wu *et al.* developed several Bell inequalities in terms of both probabilities and correlation functions for three qubits, which can be numerically violated by any pure entangled state [35, 36]. Recently, a more significant progress was achieved by K. Chen *et al.* [28]. They presented a family of Bell inequalities involving only two measurement settings of each observer for $N > 2$ qubits, which is violated by any N-qubit generalized GHZ state, and moreover the amount of maximal violation grows exponentially as $2^{(N-2)/2}$.

There are much work on the theoretical aspect, whereas no experiments aim to display so far. In this paper, we simulate the violation of two different Bell-type inequalities, i.e., MABK inequality [5] and Chen's inequality [28], for a three-qubit GHZ state as well as for generalized GHZ states in an NMR system. The experimental results clearly shows that the high efficiency of Chen's inequality and the limitation of MABK inequalitytfor any generalized GHZ entangled states . Our experimental results are well coincident with the prediction of quantum mechanics.

II.Simulation violation of MABK inequality for GHZ state

Let us consider such a scenario: there are three observers Alice (A), Bob (B), and Charlie (C), each having one qubit. The formulation of the MABK inequality is based on the assumption that every observer is allowed to choose one observable between two dichotomic observables. Denote the outcome of observer X's measurement by $X_i, X = A, B, C$, with $i = 1, 2$. Under the assumption of local realism, each outcome can either take value $+1$ or -1. In a specific run of the experiment, the correlations between the measurement outcomes of all three observers can be represented by the product $A_iB_jC_k$, where $i, j, k = 1, 2$. In a local realistic theory, the correlation function of the measurements performed by all three observers is the average of $A_iB_jC_k$ over many runs of the experiment, The MABK inequality reads as [5]

$$\begin{aligned} | \quad & E(A_1, B_2, C_2) + E(A_2, B_1, C_2) + \\ & E(A_2, B_2, C_1) - E(A_1, B_1, C_1)| \leq 2. \end{aligned} \tag{2}$$

We denote the left-hand side of the MABK inequality by $|\mathcal{B}_{MABK}|$ where $-2 \leq \mathcal{B}_{MABK} \leq 2$. In any local hidden variable (LHV) theory, the absolute value of a particular combination of correlations is bounded by 2. However, if one turns to quantum mechanics, this inequality can be violated. For MABK inequality, the maximal violation allowed by quantum mechanics is 4 [30], which for standard GHZ state,

$$|\Phi\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle). \tag{3}$$

To prepare standard GHZ state from $|000\rangle$, we used the network as shown in Fig.1, by selecting the rotation angle $2\theta = \pi/2$. After that, we will measure the spin projection $\boldsymbol{\sigma}\cdot\boldsymbol{n}$, where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector form of Pauli matrices and the two measurement directions for every qubit we chose here are $\boldsymbol{n_1} = (1, 0, 0)$ and $\boldsymbol{n_2} = (\cos\alpha, \sin\alpha, 0)$.

For this special spin projection measurement, the theoretical result of $\mathcal{B}_{MABK}$ is (for convenience we just ignore the absolute value sign)

$$\mathcal{B}_{MABK} = 3(\cos^2\alpha - \sin^2\alpha) - 1, \tag{4}$$

demonstrating that for $\alpha = 0.3041\pi \sim 0.6959\pi$ the result violates MABK inequality and reach the maximal violation value 4 when $\alpha = \pi/2$, as shown in Fig.4.

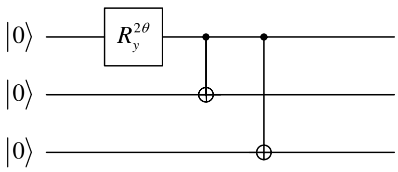


FIG. 1: Quantum network for creating a generalize GHZ state. The initial state is $|000\rangle$. After rotating qubit 1 by the angle 2θ about Y axis, we get $\cos\theta\,|000\rangle + \sin\theta\,|100\rangle$.Then through two control gates CNOT_{12} and CNOT_{13}, a generalize GHZ state $\cos\theta\,|000\rangle + \sin\theta\,|111\rangle$ will be created.

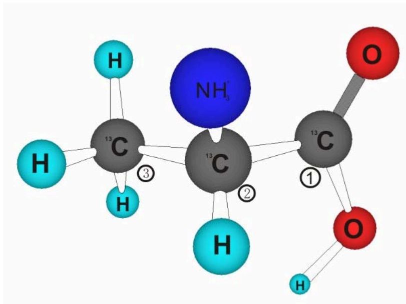
For NMR experimental implementation, there are still two problems to be solved. Firstly, the thermal equilibrium state of a NMR system at room temperature is highly mixed. We can use pseudo-pure state(PPS) [31] technique to overcome this, that the initial state is transformed to

$$\rho_{pps} = \frac{(1-\varepsilon)}{2^n} I_{2^n} + \varepsilon\,|\varphi\rangle\,\langle\varphi|\,, \tag{5}$$

which is a mixture of the totally mixed state I_{2^n} unchanged when applying with unitary transformations and a pure state $|\varphi\rangle$ which we set to be $|0\rangle$ in our experiment with the polarization $\varepsilon = 10^{-5} \sim 10^{-6}$. So ignoring I_{2^n} which does not affect NMR experiments and using the entanglement(strictly, pseudo-entanglement) of the pure part, we can simulate violation of the Bell-type inequalities we mentioned in this letter. Another problem is only the spin projection values under computational basis can be directly measured. The solution is to rotate the state or density matrix instead of changing the projective direction,

$$\begin{aligned} M = Tr(\rho \cdot M_1) &= Tr(\rho \cdot U^+ M_2 U) \\ &= Tr(U\rho U^+ \cdot M_2), \end{aligned} \tag{6}$$

where M_1 and M_2 are the desired and experimental measurements, respectively. U is one unitary operation satisfying $M_1 = U^+ M_2 U$. In NMR experiments we can apply U to the density matrix and then perform measurement of M_2, which is equivalent to measuring M_1.



	C1	C2	C3
C1	17740 Hz		
C2	53.98 Hz	5128.2 Hz	
C3	-1.18 Hz	34.88 Hz	1676.7 Hz

FIG. 2: Molecular structure and Hamiltonian parameters for alanine. The diagonal elements are the chemical shifts of the three carbon nuclei and the off-diagonal elements are the J-coupling strengths.

All experiments were performed at room temperature on a Bruker Avance 400MHz NMR spectrometer. We used the spins of three ^{13}C nucle in alanine dissolved in D_2O. The system Hamiltonian can be written as

$$H_{sys} = \sum_{i=1}^{3} \omega_i I_z^i + 2\pi \sum_{i<j}^{3} J_{ij} I_z^i I_z^j, \tag{7}$$

with the Larmor angular frequencies ω_i in the rotating frame and J-coupling constants J_{ij}, whose values are listed in Fig.2.

The whole experiment was divided into three steps. Firstly, to prepare ρ_{pps} from the thermal equilibrium state by using the spatial average technique [32]. Secondly, to prepare a standard GHZ state by using the network in Fig. 1 with $2\theta = \pi/2$. Finally, to rotate the required qubits and execute the projective measurements.

In order to improve the accuracy of radio frequency (RF) pulses, we used strongly modulating pulse (SMP) techniques [33]. We also maximized the effective gate fidelity by averaging over a weighted distribution of RF field strengths to overcome the inhomogeneity of the RF fields over the sample. The gate fidelity we calculated for every pulse is higher than 0.995 considering the RF field inhomogeneity. The range of the pulse lengths are about from $200 \sim 700\mu s$.

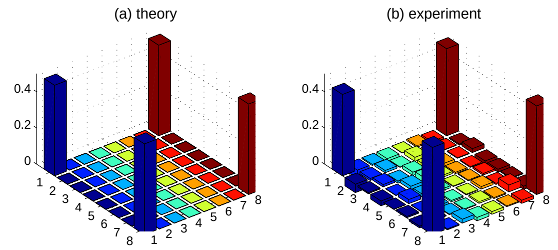


FIG. 3: Theoretical (a) and experimental (b) density matrices of the standard GHZ state $(|000\rangle + |111\rangle)/\sqrt{2}$.

Fig.3 (b) shows a full state tomography of the standard GHZ state prepared in experiment. The overall fidelity is

$$F = \frac{Tr(\rho_{th}\rho_{exp})}{\sqrt{(Tr(\rho_{th}^2)Tr(\rho_{exp}^2))}} = 0.98, \tag{8}$$

We took several sets of observers to do the corresponding measurement on standard GHZ state. The experimental result is shown in the Fig.4, where the blue squares stand for the experiment results, and the red thick line stands for the theoretical result. Clearly, the experiment results are in excellent agreement with the theoretical expectation of quantum mechanics.

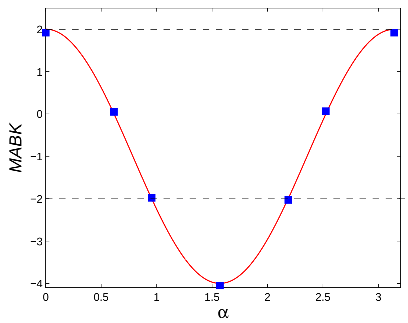


FIG. 4: $\mathcal{B}_{MABK}$ as a function of α. The red thick line stands for the theoretical expectation, and the blue square stands for the experimental data.

III. Simulation violation of MABK inequality for generalize GHZ states

So far, almost all previous Bell experiments were performed on maximal entangled states, such as Bell states and standard GHZ states. Recently, sorts of unexpected properties about nonmaximal entangled states have been shown[26, 27]. Therefore, we will next simulate the violation of MABK inequality for generalized GHZ states.

In this experiment, we choose the directions of the two measurements for every particles are $\boldsymbol{n_1} = (1, 0, 0)$ and $\boldsymbol{n_2} = (0, 1, 0)$. For these special spin projection measurements, the theoretical result of $\mathcal{B}_{MABK}$ for generalized GHZ states satisfies such a function,

$$|\mathcal{B}_{MABK}| = |-4\sin(2\theta)|. \tag{9}$$

From (9), one can see that the maximal violation is obtained when $\theta = \frac{\pi}{4}$ just the standard GHZ state. Obviously, the MABK inequality is efficient only in the region of $\theta \in [\frac{\pi}{12}, \frac{5\pi}{12}]$; in other words, only in such region the inequality can be violated.

We measured a set of generalized GHZ states with particular angle θ. The result is shown in Fig.5 which shows a good consistence with the prediction of quantum theory.

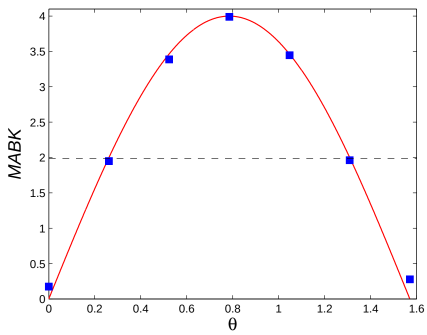


FIG. 5: The values of $\mathcal{B}_{MABK}$ as a function of θ. The red thick line stands for the theoretical expectation, and the blue squares stand for the experiment data.

IV. Simulation violation of Chen's inequality for generalize GHZ states

For a three-qubit system, Chen's inequality can be written as

$$\begin{aligned}\mathcal{B}_{Chen} = \frac{1}{2}(&E(A_1, B_1, C_1) + E(A_1, B_2, C_1) + E(A_2, B_1, C_1) - E(A_2, B_2, C_1) + E(A_1, B_1, C_2) + \\ &E(A_1, B_2, C_2) + E(A_2, B_1, C_2) - E(A_2, B_2, C_2)) + E(C_1) - E(C_2),\end{aligned} \tag{10}$$

$|\mathcal{B}_{Chen}| \leq 2$ in the LHV model.

In experiment, based on [29], we take the directions of two measurement about A and B as $\boldsymbol{n_1} = (1, 0, 0)$ and

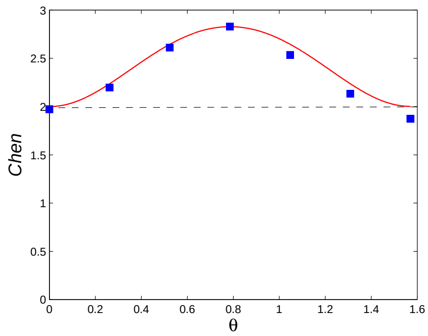


FIG. 6: The values of $\mathcal{B}_{Chen}$ as a function of θ. The red thick line stands for the theoretical result, and the blue square stands for the experiment result.

$\boldsymbol{n_2} = (0, 1, 0)$. For C, the directions of two measurement are $\boldsymbol{n_1} = (\sin\alpha\cos(-\frac{\pi}{4}), \sin\alpha\sin(-\frac{\pi}{4}), \cos\alpha)$ and $\boldsymbol{n_2} = (\sin(\pi-\alpha)\cos(-\frac{\pi}{4}), \sin(\pi-\alpha)\sin(-\frac{\pi}{4}), \cos(\pi-\alpha))$, where

$$\begin{aligned} \alpha &= \tan^{-1}[\sqrt{2}\tan(2\theta)], & 0 \leq \theta \leq \frac{\pi}{4} \\ \alpha &= \tan^{-1}[\sqrt{2}\tan(2\theta)] + \pi, & \frac{\pi}{4} \leq \theta \leq \frac{\pi}{2} \end{aligned} \quad (11)$$

Then, we obtain $\mathcal{B}_{Chen}$ as

$$\mathcal{B}_{Chen} = 2[2\sin^2(2\theta) + \cos^2(2\theta)]^{1/2}. \quad (12)$$

The results are always larger than 2 no matter whatever θ is. It illustrates that, the whole region of generalized GHZ states can violate the inequality by a set of suitable observation angles.

Obviously, Chen's inequality is more efficient than MABK inequality for generalized GHZ states. The experimental result is shown in Fig.6, which perfectly simulates the violation of Chen's inequality for generalize GHZ states. It shows that our experimental result is in good agreement with quantum mechanical theory.

V. Conclusions

In summary, we have investigated the simulation of the violation of Bell-type inequalities, including MABK inequality and Chen's inequality for a three-qubit GHZ state as well as the generalized GHZ states in a NMR system. In the range of the generalized GHZ states, these experiments shows that Chen's inequality is more efficient than MABK inequality. The experimental results are well in agreement with the expectation of quantum mechanics.

It is necessary to emphasize that, in strict, because NMR qubits are many nuclear spins of atoms bounded together in a single molecule, separated by a few angstroms, the NMR experiment is inherently local. That is to say, our results are also consistent with the classical theory,depending on whether we have considered the mixed part I_{2^n}. Whereas, the meaning is that, when we experimentally simulate the violation of different Bell-type inequalities for arbitrary generalized three-qubit GHZ states in NMR, the results excellently display the quantum predictions. It tells us, despite of many existed disputes, NMR may contribute more on some fundamentals of quantum mechanics. As a refined tool and technique for experimentally realizing quantum computation in the last decade, NMR is still contributing to numerous fundamental problems of quantum mechanics now. In the future, we will still pay attention to this area.

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[1] J. S. Bell, Physics (Long Island city, N.Y) 1,195 (1964).
[2] H. P. Stapp, Nuovo Cimento Soc. Ital. Fis. B 29, 270 (1975).
[3] M. Żukowski, Stud. Hist. Phil. Mod. Phys. 36, 566 (2005).
[4] J. Clauser, M. Horne, A. Shimony, and R. Holt, Phys. Rev. Lett. 23, 880 (1969).
[5] N. D. Mermin, Phys. Rev. Lett. 65, 1838 (1990); S. M. Roy and V. Singh, ibid. 67, 2761 (1991); M. Ardehali, Phys. Rev. A 46, 5375 (1992); A. V. Belinskii and D. N. Klyshko, Phys. Usp. 36, 653 (1993); N. Gisin and H. Bechmann-Pasquinucci, Phys. Lett. A 246, 1 (1998).
[6] R. F. Werner and M. M. Wolf, Phys. Rev. A 64, 032112 (2001); M. Żukowski and Č Brukner, Phys. Rev. Lett. 88, 210401 (2002).
[7] Č Brukner, M. Żukowski, J. W Pan, and A. Zeilinger, Phys. Rev. Lett. 92, 127901 (2004).
[8] G. Brassard, H. Buhrman, N. Linden, A. A. Mthot, A. Tapp, and F. Unger, Phys. Rev. Lett. 96, 250401 (2006).
[9] V. Scarani, and N. Gisin, Phys. Rev. Lett. 87, 117901 (2001).
[10] Z. B. Chen, Q. Zhang, X. H Bao, J. Schmiedmayer and J. W. Pan, Phys. Rev. A 73, 050302 (2006).
[11] A. Acín, N. Gisin, and L. Masanes, Phys. Rev. Lett. 97, 120405 (2006).
[12] J. Barrett, L. Hardy, and A. Kent, Phys. Rev. Lett. 95, 010503 (2005).
[13] A. Acín, N. Brunner, N. Gisin, S. Massar, S. Pironio, V. Scarani, Phys. Rev. Lett. 98, 230501 (2007).
[14] M. A. Nielsen, and I. L. Chuang, Quantum Computation and Quantum Information (Cambridge: Cambridge University Press) (2000).
[15] S. J. Freedman and J. F. Clauser, Phys. Rev. Lett. 28, 938 (1972).
[16] A. Aspect, J. Dalibard, and G. Roger, Phys. Rev. Lett. 49, 1804 (1982).
[17] G. Weihs et al., Phys. Rev. Lett. 81, 5039 (1998).
[18] D. L. Moehring et al., Phys. Rev. Lett. 93, 090410 (2004).
[19] D. N. Matsukevich et al., Phys. Rev. Lett. 95, 040405 (2005).
[20] D. N. Matsukevich et al., Phys. Rev. Lett. 100, 150404 (2008).
[21] D. N. Matsukevich et al., Phys. Rev. Lett. 96, 030405 (2006).
[22] C.-W. Chou et al., Science 316, 1316 (2007).
[23] M. A. Rowe et al., Nature (London) 409, 791 (2001).

[24] A. M. Souza et al., New. J. Phys. 10, 033020 (2008).
[25] C. Y. Lu, (private communication).
[26] A. Acín,, T. Durt, N. Gisin and J. I. Latorre, Phys. Rev. A 65, 052325 (2002).
[27] A.A. Méthot and V. Scarani, Quant. Inf. Comput. 7, 157 (2007).
[28] K. Chen, S. Albeverio, and S. M. Fei, Phys. Rev. A 74, 050101(R)(2006).
[29] M. S. Anwar , D. Blazina *et.al*, Phys. Rev. Lett. 93, 040501 (2004).
[30] V. Scarani and N. Gisin, J. Phys. A 34, 6043 (2001).
[31] N. A. Gershenfeld, I. L. Chuang, Science 275, 350-356 (1997).
[32] D. G. Cory, A. F. Fahmy and T. F. Havel, Proc. Natl. Acad, Sci. USA, 94:1634 (1997).
[33] E. Fortunato *et al.*, Chem. Phys. 116(17), 7599 (2002).
[34] M. Żukowski, Č Brukner, W. Laskowski, and M. Wiesniak, Phys. Phys. Rev. Lett. 88, 210402 (2002).
[35] J. L. Chen, C. F. Wu *et al.*, Phys. Rev. Lett. 93, 140407 (2004).
[36] C. F. Wu, J. L. Chen *et al.*, Phys. Rev. A 77, 062309 (2008).