Simulation of Bell-type inequalities violation for three qubits in 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, the tests of different Bell's inequalities, MABK inequality and Chen's inequality are also carried out. The experimental results display that MABK inequality is inefficienct in a region of generalized GHZ states. However, Chen's inequality is efficienct 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 is easily found that entangled states violate these inequalities in quantum mechanics. From these inequalities, the crucial conflict between classical theory and quantum mechanics is shown. 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]. Recently, there has been increasing interest in the subject of Bell's inequalities, not only to test foundation problems of quantum mechanics, but also because of 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 NMR system [24].

In this paper, we simulate the violation of Bell-type inequalities for three-qubit GHZ state in NMR system. Furthermore, we also simulate the violation of Bell-type inequalities for generalized GHZ states in NMR system. Previous experiments mainly focused on the maximal entangled states, such as Bell state, standard GHZ state, etc, rarely on nonmaximal entangled states, such as generalized GHZ states. The reason is, such as in photon experiments, preparing a nonmaximal entangled state is as difficult as standard GHZ state. Researchers generally consider it is not worth the candle in photon system [25]. On the other hand, there are many phenomena disclosed by nonmaximal entangled states, for instance, the nonmaximal entangled states make lots of Bell-type inequalities arrive the maximal violation [26, 27]. There are still many open problems about nonmaximal entangled states. Especially, as the number of particle increasing, it may exhibit unexpected properties. Therefore, it is interesting and meaningful to study the nonmaximal entangled states.

For generalized GHZ states, Scarani and Gisin [30] firstly found that there exist a region of three-qubit generalized GHZ states (8) satisfy the MABK inequality. It is shown that for $\theta \leq \pi/12$ or $\theta \geq 5\pi/12$ the states (8) do not violate the three-qubit MABK inequality. Hence, Scarani and Gisin deduced that MABK inequalities and more generally the family of Bell's inequalities with two observables per qubit, may not be the 'natural' generalizations of the CHSH inequality to more than two qubits [30]. Whereafter, a set of multipartite Bell inequalities has been elegantly derived, which is the WWZB inequality [6]. Actually, The WWZB inequalities include MABK inequalities as special cases. Furthermore, Żukowski *et.al* proved and showed that [34] (i)for $N = even$, although the generalized GHZ state does not violate MABK inequalities, it violates the WWZB inequality, and (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. As to obtain such a Bell-type inequality involving only two measurement settings per observer, which is violated by the generalized GHZ state in the whole region of θ for any number of qubits, several notable work were shown. Chen and Wu *et al.* developed several Bell inequalities in terms of both probabilities and correlation functions for three qubits, which can be seen numerically to be violated by any pure entangled state [35, 36]. Recently, a more significant progress derived 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 not only violated by the N-qubit generalized GHZ state in the whole

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region,but also the amount of maximal violation grows exponentially as $2^{(N-2)/2}$.

From the above description in theory, more efficient Bell-type inequalities for generalized GHZ states are derived. However, no experiments aim to display so far. Therefore, we simulate tests for different Bell's inequalities, MABK inequality [5] and Chen's inequality [28]in NMR system. The experimental results obviously display that MABK inequality is inefficient in a region of generalized GHZ states. However, Chen's inequality is efficient for any generalized GHZ entangled states. The facts proved that all of our experimental results are coincident with the prediction of quantum mechanics.

The content of this paper is organized as follows. In Sec. II, we introduced the experiment about violation of MABK inequality for standard three-qubit GHZ state in NMR system. Furthermore, In Sec. III, we simulate the violation of MABK inequality for generalized GHZ states. In Sec. IV, the experimental results of simulating the violation of Chen's inequality for generalized GHZ states were derived. Finally, we summarize and discuss our results.

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 based on the assumption that every observer is allowed to choose 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 [5]

$$\begin{aligned} | \quad & E(A_1, B_2, C_2) + E(A_2, B_1, C_2) + \\ & E(A_2, B_2, C_1) - E(A_1, B_1, C_1)| \leq 2. \end{aligned} \tag{1}$$

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,

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

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 $\boldsymbol{\sigma \cdot n}$, 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)

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

displaying 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.

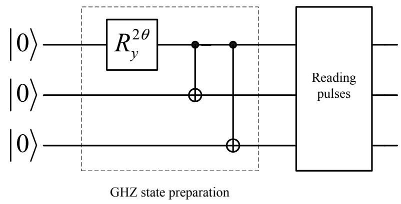


FIG. 1: A quantum network for creating a generalize GHZ state. The initial state is $|000\rangle$. After rotating qubit 1 by the angle 2θ about Y axis, we get $\cos\theta|000\rangle + \sin\theta|100\rangle$.Then through two control gates CNOT_{12} and CNOT_{13}, a generalize GHZ state $\cos\theta|000\rangle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

$$\rho_{pps} = \frac{(1-\varepsilon)}{2^n} I_{2^n} + \varepsilon|\varphi\rangle\langle\varphi|, \tag{4}$$

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 we can rotate the state or density matrix instead of changing the projective direction,

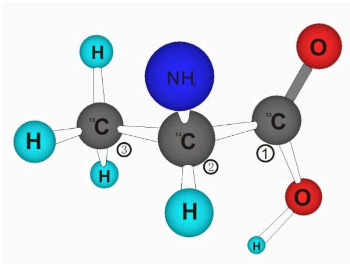
$$\begin{aligned} M = Tr(\rho \cdot M_1) &= Tr(\rho \cdot U^+ M_2 U) \\ &= Tr(U\rho U^+ \cdot M_2), \end{aligned} \tag{5}$$

where M_1 and M_2 is the desired measurement and experimental measurement, 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.

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

$$H_{sys} = \sum_{i=1}^{3} \omega_i I_z^i + 2\pi \sum_{i<j}^{3} J_{ij} I_z^i I_z^j, \tag{6}$$

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



	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.

The whole experiment was divided into three steps. Firstly, to prepare ρ_{pps} from the thermal equilibrium state, using the spatial average technique [32]. Secondly, to prepare a standard GHZ state, we use a Hardmard gate and two CNOT gates, that is to say, set $\theta = \pi/2$ in Fig.1. Finally, to rotate the required qubits and execute the projective measurements.

In order to improve the accuracy of radio frequency (RF) pulses, we use strongly modulating pulse (SMP) techniques [33] to simulate the theoretical unitary operations. We also maximize 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 (b) shows a full state tomography of the standard GHZ state in experiment. The overall fidelity is

$$F = \frac{Tr(\rho_{th}\rho_{exp})}{\sqrt{(Tr(\rho_{th}^2)Tr(\rho_{exp}^2))}} = 0.98, \tag{7}$$

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

Of course, if we had considered the huge mixed state I_{2^n} into the experiment, we would get the result in agreement with the classical theory. Therefore, this is why we emphasize that the experiments are simulation not proof.

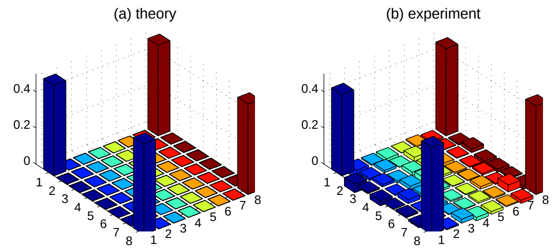


FIG. 3: Theoretical (a) and experimental (b) density matrices of the standard GHZ state $(|000\rangle+|111\rangle)/\sqrt{2}$. The bars' height at the four vertices of the density matrix is 0.5 theoretically, respectively. The fidelity is 0.98.

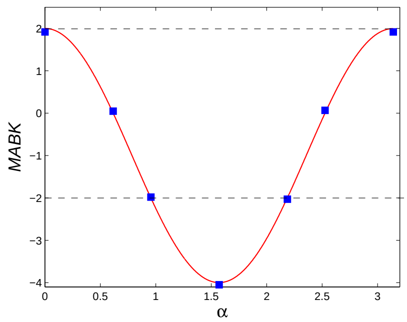


FIG. 4: $\mathcal{B}_{MABK}$ as a function of α. The red thick line stands for the theoretical expectation, and the blue square stands for the experimental data.

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 state and standard GHZ state. Recently, sorts of unexpected properties about nonmaximal entangled states have been shown[26, 27]. Therefore, we simulate the violation of MABK inequalities for generalized GHZ states in NMR system further. The generalized GHZ states can be expressed as

$$|\Psi\rangle = \cos\theta\,|000\rangle + \sin\theta\,|111\rangle\,. \tag{8}$$

which $\theta \in [0, \frac{\pi}{2}]$.

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 only in the region of

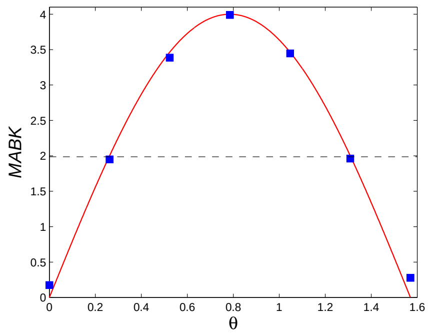


FIG. 5: The values of $\mathcal{B}_{MABK}$ as a function of θ. The red thick line stands for the theoretical expectation, and the blue squares stand for the experiment data.

$\theta \in [\frac{\pi}{12}, \frac{5\pi}{12}]$ is efficient, in other words, only in such region the inequality can be violated. Therefore, MABK inequality is not efficient in the whole region of generalized GHZ states.

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

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

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

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

$|\mathcal{B}_{Chen}| \leq 2$ 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 $\boldsymbol{n_2} = (0,1,0)$. 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

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

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

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

The results are always larger than 2 no matter whatever

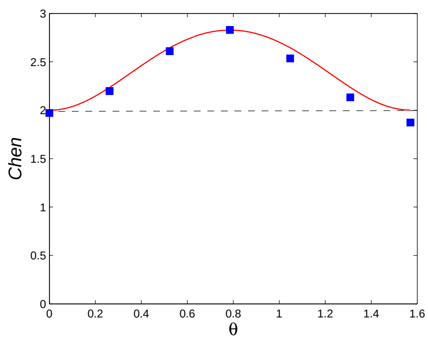


FIG. 6: The values of $\mathcal{B}_{Chen}$ as a function of θ. The red thick line stands for the theoretical result, and the blue square stands for the experiment result.

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 is shows that our experimental result is in good agreement with quantum mechanical theory.

V. Conclusions

In summary, we have simulated the experimental violation of MABK inequalities for a three-qubit GHZ state in a NMR system. Furthermore, we focus on the nonmaximal entangled states, the violation of MABK inequality for generalized states in NMR system are shown. The experimental results are well in agreement with the expectation of quantum mechanics. As to exhibit test of different Bell-type inequality for generalized GHZ states, we also simulated Chen's inequality. Comparing these two results, it shows that MABK inequality is not efficient in the whole region of generalized GHZ states. While, Chen's inequality is efficient for any generalized GHZ entangled state. The facts proved that all of our experimental results are coincident with the prediction 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 an NMR experiment is inherently local. Our results are also in good agreement with the local hidden variable theory. It may appear puzzled that quantum and classical theory are both consistent with our experiments.

However, it can be understood, although the entire system is local, NMR is only sensible for the deviation part of the mixed state, which behaves like a "pure entangled state". Hence, our experiments in NMR system do not really prove the violation of Bell-type inequalities. This is why we always explain that our experiments are simulation not proof. 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 system, the results excellently display the quantum predictions. It tells us, despite of existed many disputes, NMR systems may contribute more on some fundamentals of quantum mechanics. After all, it is less exploited experimentally outside the scope of optics. Besides, if our experiments were carried out in a highly polarized spin ensemble [29], true entangled states can be achieved and contradiction between hidden variables models and quantum theory could be detected. As a refined tool and technique for experimentally realizing quantum computation in the last decade, NMR is still contributing to many fundamental problems of quantum mechanics now. In the future, we will still pay attention to this area.

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