II.simulating 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,

$$E(A_i, B_j, C_k) =< A_iB_jC_k >_{avg} . \tag{1}$$

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 [24], by the standard GHZ state, i.e., the state with $\theta = \frac{\pi}{4}$ in Eq. (**??**). As an example, in this section, we simulated the violation of MABK inequality for the standard GHZ state.

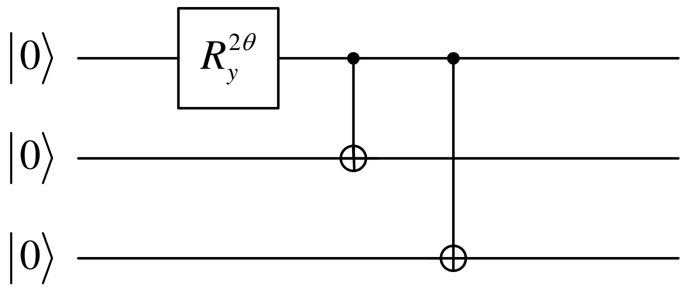

FIG. 1: Quantum network for creating a generalized GHZ state. The input state is $|000\rangle$. $R_y^{2\theta}$ denotes a rotation of an angle 2θ along Y axis, following by two controlled-not (CNOT) gates. The output state is a generalized GHZ state $\cos\theta\,|000\rangle + \sin\theta\,|111\rangle$.

To prepare standard GHZ state from $|000\rangle$, we used the network as shown in Fig.1, by selecting the rotation angle $\theta = \pi/4$. 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 $\boldsymbol{n_2} = (\cos\alpha, \sin\alpha, 0)$. In other words, the two dichotomic observables allowed to be chosen for A,B,C are $\boldsymbol{\sigma_{n_1}}$ and $\boldsymbol{\sigma_{n_2}}$.

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

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

demonstrating that for $\alpha = 0.3041\pi \sim 0.6959\pi$, $\mathcal{B}_{MABK} > 2$ to violate MABK inequality and reach the maximal violation value 4 when $\alpha = \pi/2$.

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) [29] technique to overcome this. Instead of a pure state $|000\rangle$, we prepared a PPS:

$$\rho_{pps} = \frac{(1-\varepsilon)}{2^n} I_{2^n} + \varepsilon \left|000\right\rangle \left\langle 000\right| . \tag{4}$$

It is a mixture of the totally mixed state I_{2^n} unchanged when applying with unitary transformations and a pure state $|000\rangle$ with the polarization $\varepsilon \approx 10^{-5}$. 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. The second problem is only the spin projection values under a computational basis can be directly measured. The solution is to rotate the state or density matrix instead of changing the projective direction,

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

where M_1 and M_2 are the desired and experimental measurements, respectively. U is one unitary operation satisfying $M_1 = U^\dagger M_2 U$. 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

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

with the resonance frequencies ω_i and J-coupling constants J_{ij}. The chemical shifts of the three carbon nuclei are $\omega_1 = 5128.2Hz$, $\omega_2 = 17740Hz$, and $\omega_3 = 1676.7Hz$; the J-coupling strengths are $J_{12} = 53.98Hz$, $J_{23} = -1.18Hz$, and $J_{13} = 34.88Hz$.

The whole experiment was divided into three steps. Firstly, to prepare ρ_{pps} from the thermal equilibrium state by using the spatial average technique [30]. Secondly, to prepare a standard GHZ state by using the network in Fig. 1 with $\theta = \pi/4$. 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 [31]. 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 $200 \sim 700\mu s$.

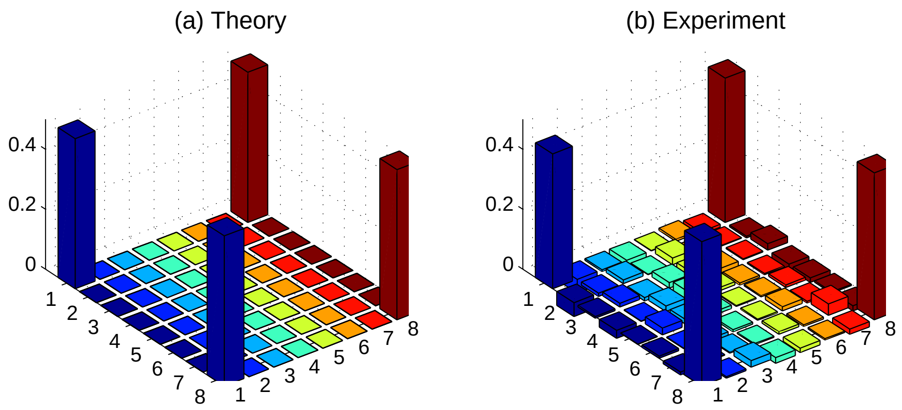

FIG. 2: Theoretical (a) and experimental (b) density matrices of the standard GHZ state $(|000\rangle + |111\rangle)/\sqrt{2}$.

Fig.2 (b) shows a full state tomography of the standard GHZ state prepared in experiment. The overall fidelity is

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

We took the observers mentioned above $(\boldsymbol{\sigma_{n_1}}, \boldsymbol{\sigma_{n_2}})$ to do the corresponding measurement on the standard GHZ state. The experimental result is shown in Fig.3, where the blue squares stand for the experiment results, and the red thick line stands for the theoretical result. Clearly, the experimental results are in excellent agreement with the theoretical expectation of quantum mechanics.

III. Simulating violation of MABK inequality for generalized GHZ states

So far, almost all previous Bell experiments were performed on maximal entangled states, such as Bell state and the standard GHZ state. Recently, much work about nonmaximal entangled states have been done[22, 23]. In this

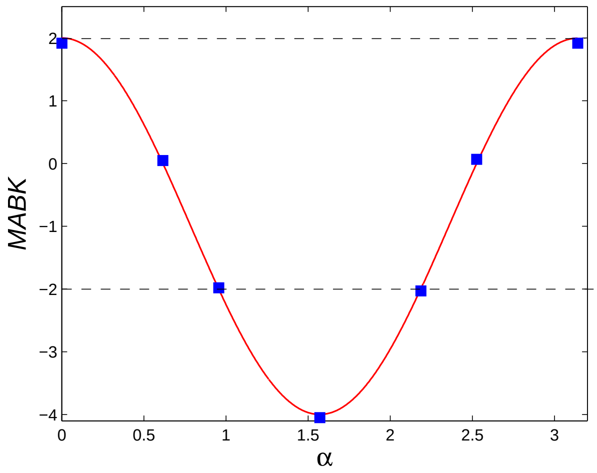

FIG. 3: Experimental test of the MABK inequality for a standard GHZ state. The red thick line stands for the theoretical expectation, and the blue square stands for the experimental data.

section, we simulated the violation of MABK inequality for the generalized GHZ state.

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

$$|\mathcal{B}_{MABK}| = | - 4\sin(2\theta)|. \tag{8}$$

From Eq. (8), 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 a region the inequality can be violated.

We measured a set of generalized GHZ states with particular angles θ. Fig.4(a) shows the experimental date along with the theoretical expectation.

IV. Simulating violation of Chen's inequality for generalized GHZ states

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

$$\mathcal{B}_{Chen} = \frac{1}{2}(E(A_1, B_1, C_1) + E(A_1, B_2, C_1) + E(A_2, B_1, C_1) - E(A_2, B_2, C_1) + E(A_1, B_1, C_2) + E(A_1, B_2, C_2) + E(A_2, B_1, C_2) - E(A_2, B_2, C_2)) + E(C_1) - E(C_2), \tag{9}$$

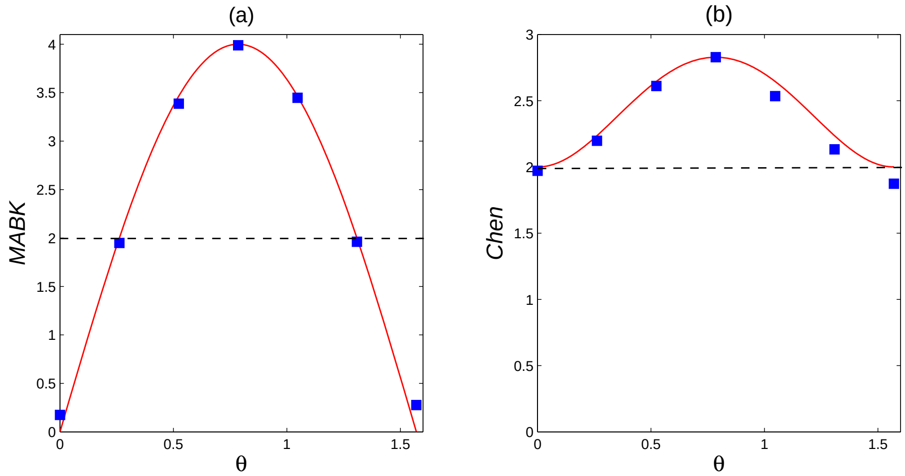

FIG. 4: For the generalized GHZ states, (a) the values of $\mathcal{B}_{MABK}$ as a function of θ, (b) the values of $\mathcal{B}_{Chen}$ as a function of θ. The red thick line stands for the theoretical expectation, and the blue square stands for the experiment data.

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

In experiment, we took 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 were chosen as $\boldsymbol{n_1} = (\sin\alpha\cos(-\frac{\pi}{4}), \sin\alpha\sin(-\frac{\pi}{4}), \cos\alpha)$ and $\boldsymbol{n_2} = (\sin(\pi - \alpha)\cos(-\frac{\pi}{4}), \sin(\pi-\alpha)\sin(-\frac{\pi}{4}), \cos(\pi-\alpha))$, where

$$\begin{aligned} \alpha &= \tan^{-1}[\sqrt{2}\tan(2\theta)], \qquad & 0 \leq \theta \leq \frac{\pi}{4} \\ \alpha &= \tan^{-1}[\sqrt{2}\tan(2\theta)] + \pi, \qquad & \frac{\pi}{4} \leq \theta \leq \frac{\pi}{2} \end{aligned} \tag{10}$$

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

$$\mathcal{B}_{Chen} = 2[2\sin^2(2\theta) + \cos^2(2\theta)]^{1/2}, \tag{11}$$

which tells us that $\mathcal{B}_{Chen}$ always larger than 2 no matter whatever θ is. It illustrates that, the whole region of the 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.4(b), which perfectly simulates the violation of Chen's inequality for the generalize GHZ states.

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