Bell Inequality Violations in a Liquid NMR System

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Two violations of Bell inequalities are tested in a two-qubit liquid NMR system. Violation of the CHSH two-qubit correlation inequality is observed in a cat state, but not in a pure state. Violation of the single-qubit Leggett-Garg time inequality is observed in a mixed state using a CNOT gate to perform non-invasive measurements.

I. INTRODUCTION

Under a hidden variable interpretation of quantum mechanics, particles that appear to be in a superposition of states are secretly in a single state. A deeper understanding of the system or of physics could reveal these hidden variables, which would enable measurement of properties with greater precision than allowed by the uncertainty principle. Albert Einstein was among the most well known proponents of this interpretation, stating his belief that "[God] does not play dice with the universe".

However, in 1964, Bell [1] realized that in certain cases, having different observers measure correlated quantities leads to quantum mechanical predictions that violate assumptions of hidden variable theories. Specifically, quantum mechanics predicts that the only way to preserve hidden variables that encode the "true" state of a system is to transfer information faster than the speed of light.

Here, two experiments that demonstrate this property are investigated. The first, developed by Clauser, Horne, Shimony, and Holt (CHSH) [2] in 1969, considers the correlation between spins measured along different axis. The second, developed by Leggett and Garg [3] in 1985, asks whether measurements can be made without effecting subsequent dynamics of the system.

II. THEORY

II.1. CHSH Inequality

In the CHSH inequality, two particles a and b, each of which is a two-state system where $a, b = \pm 1$, are each observed in two reference frames (a, a' and b, b'). The four correlations between the two particles are measured, and the $CHSH$ quantity is given by

$$CHSH = E(a,b) + E(a',b) - E(a,b') + E(a',b') \quad (1)$$

If some hidden variable λ exists and determines the state of the particles, the correlation function is given by $E(a,b) = \int \overline{A}(a,\lambda)\overline{B}(b,\lambda)p(\lambda)d\lambda$, where $\overline{A}$ and $\overline{B}$ are the average values of A and B, and have a magnitude at most one. Then,

$$E(a,b) - E(a,b') = \int [\overline{A}(a,\lambda)\overline{B}(b,\lambda) - \overline{A}(a,\lambda)\overline{B}(b',\lambda)]p(\lambda)d\lambda$$

This can be written to include the other two reference frames:

$$E(a,b) - E(a,b') = \int \overline{A}(a,\lambda)\overline{B}(b,\lambda)[1 \pm \overline{A}(a',\lambda)\overline{B}(b',\lambda)] - \int \overline{A}(a,\lambda)\overline{B}(b',\lambda)[1 \pm \overline{A}(a',\lambda)\overline{B}(b,\lambda)]$$

The triangle inequality can be applied to get the final form of the CHSH inequality:

$$|E(a,b) + E(a',b) - E(a,b') + E(a',b')| \leq 2 \quad (2)$$

If the CHSH inequality is violated, a hidden variable theory cannot exist, unless special relativity is violated and one of the particles can instantaneously communicate to the other particle that it has been measured in a given way.

II.2. Leggett-Garg Inequality

Instead of measuring the correlation between two particles, the Leggett-Garg inequality considers the correlation between measurements of a single particle taken at different times. A binary property of a particle, like the spin, is measured at three different times $t_1 < t_2 < t_3$, and the correlation between each pair of times is measured.

Under a hidden variable theory, if t_1 and t_2 are correlated, and t_2 and t_3 are correlated, t_1 and t_3 must also be correlated. In this case, $E(t_1,t_2) + E(t_2,t_3) - E(t_1,t_2) = 1$, and in general, $E(t_1,t_2) + E(t_2,t_3) - E(t_1,t_2) \leq 1$

However, this treatment assumes that the measurement of the quantity does not change the subsequent evolution of the system, and it assumes that the system always has a definite value of ± 1. Quantum mechanics does not assume these properties, and violates this inequality.

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II.3. NMR

In an NMR system, molecules are placed in a strong magnetic field that causes them to precess with a frequency proportional to the applied magnetic field. Then, applying weak magnetic field pulses in perpendicular directions makes the spins rotate.

Neighboring atoms in a molecule interact via spin-spin coupling. If an atom's neighbor has its spin in the same direction as the external field, the first atom will be in a slightly stronger magnetic field, and its Larmor frequency will increase; if the neighbor is pointing in the opposite direction as the external field, the first atom will have a slightly lower frequency. Due to this behavior, time evolution of an NMR system can create entanglement between qubits.

The state of the NMR system is typically represented as a density matrix, with the diagonal elements representing the wavefunction of the spins.

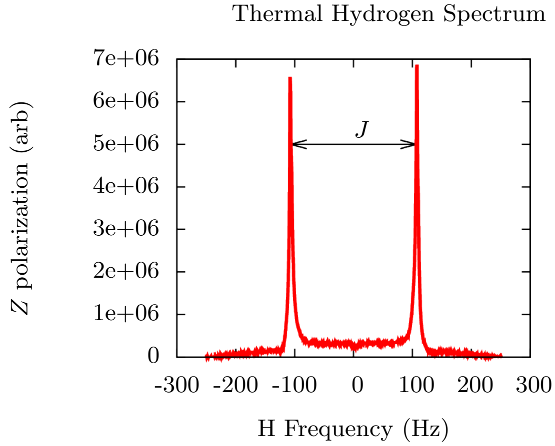

FIG. 1. Applying a 90° pulse to the hydrogen atom produces a spectrum of this form. The coupling J is given by the distance between the peaks. The size of the peaks determines $a-c$ and $b-d$, where a, b, c, d are the diagonal elements of the density matrix.

II.4. Temporal Averaging

In a liquid NMR system, most of the spins are randomly distributed, since the temperature k_BT is higher than the spin energy $\hbar\omega$. The randomness is perturbed slightly by the Hamiltonian due to the magnetic field and spin-spin coupling, which leads to the phenomena observed.

However, a zero-temperature NMR system can be simulated through a process called temporal averaging. Given the thermal state, three states that sum to

$$\begin{pmatrix}5&0&0&0\\0&3&0&0\\0&0&-3&0\\0&0&0&-5\end{pmatrix}+\begin{pmatrix}5&0&0&0\\0&-3&0&0\\0&0&-5&0\\0&0&0&3\end{pmatrix}+\begin{pmatrix}5&0&0&0\\0&-5&0&0\\0&0&3&0\\0&0&0&-3\end{pmatrix}$$
$$=\begin{pmatrix}20&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}+\begin{pmatrix}-5&0&0&0\\0&-5&0&0\\0&0&-5&0\\0&0&0&-5\end{pmatrix}$$

can be created. NMR measurements only consider traceless portions of matrices, so an effective $|00\rangle$ state is created in this way.

The use of the temporal averaging procedure creates a "detection loophole" in the Bell inequality experiments. Temporal averaging creates a non-uniform sampling of the spins in the system, which allows local realist models to describe the system being studied. In fact, a good local realist model has been developed that describes liquid NMR and predicts the same violations of Bell inequalities when temporal averaging is used[4].

III. EQUIPMENT & PROCEDURE

III.1. Spectrometer

We use a Bruker Avance 200 NMR Spectrometer prepared by the Junior Lab staff with a 7% solution of chloroform ($CHCl_3$) in a deuterated acetone solution. The spectrometer uses a large superconducting magnet to produce a strong constant B field in the z direction with a proton Larmor frequency of 200 MHz. The hydrogen and carbon atoms are used as the two qubits in this system. Magnetic field pulses can be created in the x and y directions to rotate the spins with smaller coils; these coils are also used in a superheterodyne receiver that can measure the frequency and complex phase of the signal.

To measure the state distribution of one of the qubits, a readout pulse is applied along the x axis that rotates the qubit 90° into the z axis. The spins then are allowed to precess and decay, and the Fourier transform of this free induction decay is output, as seen in Figure 1.

The FID spectrum output by the spectrometer is a function of the density matrix elements. The peaks in the hydrogen spectrum are given by $a-c$ and $b-d$. The correlation between the qubits in the $|\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$ states is 1, and -1 for $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$, so the correlation function between the two qubits is $a-b-c+d$, which is given by the difference in the two peaks in the hydrogen spectrum.

III.2. CHSH Inequality

The pseudopure states was created using a temporal averaging technique described in [5], and the cat state was created by applying a pulse sequence of the form

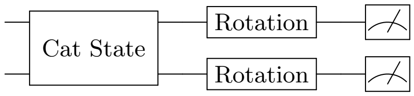

FIG. 2. Circuit used for measuring the CHSH quantity

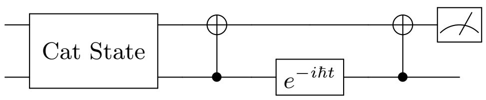

FIG. 3. Circuit used for measuring the Leggett-Garg quantity

$r_{x2}r_{x1}r'_{y2}\tau r_{y2}r'_{x1}r'_{x2}$ to a $|00\rangle$ state. The states were rotated into the appropriate bases for measuring correlation by applying r_x pulses of varying length to either qubit.

The hydrogen atom was measured in the $(0, 0, 1)$ basis and in the $(\sin 4\theta, 0, \cos 4\theta)$ basis, while the carbon atom was measured in the $(\sin 2\theta, 0, \cos 2\theta)$ basis and in the $(\sin 6\theta, 0, \cos 6\theta)$ basis. The angle θ was varied from zero to ninety degrees. The circuit used for measuring the CHSH inequality is presented in Figure 3.

III.3. Leggett-Garg Inequality

A scattering circuit [7] is used to measure the Leggett-Garg inequality. At two times, separated by either Δ or 2Δ, a CNOT gate is applied to the system, which flips the carbon atom if the hydrogen atom is in the $|1\rangle$ state. This acts as a non-invasive measurement of the hydrogen atom, and the σ_z component of the carbon atom measures the correlation between the two measurements of the hydrogen atom - if the hydrogen atom was in opposite states in each of the two measurements, the carbon atom would get flipped once and end up in the $|1\rangle$ state, and if it was in the same state in each of the two measurements, it would get flipped zero or two times, and end up back in the $|0\rangle$ state.

The delay time Δ was swept from zero to $2/J$, where J is the coupling constant between the carbon and hydrogen atoms, approximately 215 Hz.

IV. RESULTS

IV.1. CHSH Inequality

The CHSH quantity (Equation 1) was measured for the two-qubit system described in III.1. The system was first prepared in the non-entangled pure $|00\rangle$ state, then in the entangled $(|00\rangle + |11\rangle)/\sqrt{2}$ cat state. Results for the pure state, which does not violate the CHSH inequality, are given in Figure 4. Results for the cat state, which does violate the inequality, are given in Figure 5.

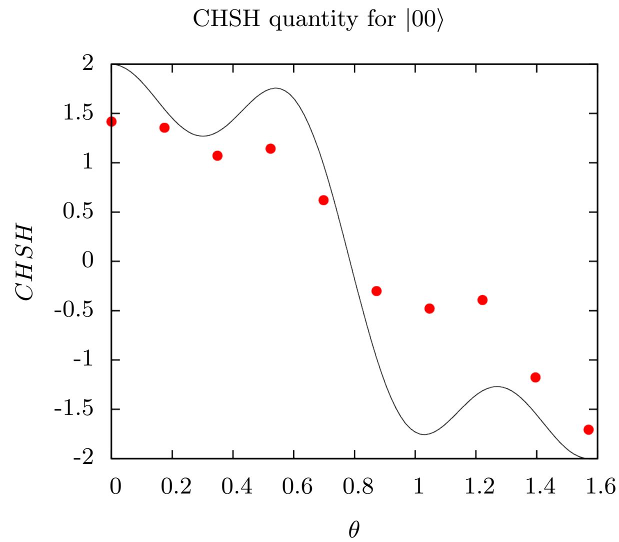

FIG. 4. For a pure state, the CHSH inequality is not violated. The magnitude of the CHSH quantity is suppressed due to pulse width inconsistencies, but the measured values have the same shape as the predicted curve.

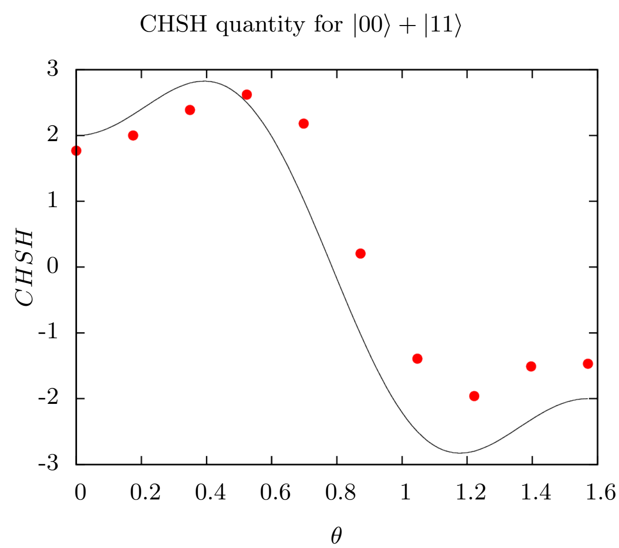

FIG. 5. In an entangled state, the CHSH quantity takes on a maximum measured value of 2.62, compared to the predicted $2\sqrt{2} = 2.83$.

Ideally, the maximum value for the cat state would be $2\sqrt{2}$, but we find a maximum value of only 2.62. We also find that the second peak of the cat state is only -1.96, and does not violate the inequality. This is likely due to magnetic field gradients and inhomogeneities in the spectrometer, as well as slightly incorrect pulse widths which cause the cat state to be non-ideal. This is further evidenced by the zero crossing in the measured data occurring at a slightly larger angle than in the prediction.

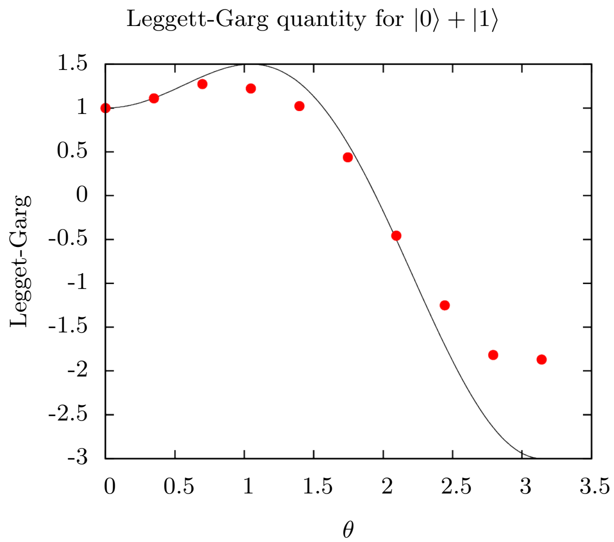

FIG. 6. When the analyzed qubit is in a mixed $|0\rangle+|1\rangle$ state, the Leggett-Garg inequality is violated with a maximum measured value of 1.27, compared to an expected value of 1.5.

	Measured	Quantum	Classical
CHSH cat state	2.62	2.83	2
CHSH pure state	1.73	2	2
Leggett-Garg mixed state	1.27	1.5	1

TABLE I. Comparison of measured inequality values to classical and quantum predictions. In the CHSH cat state and Leggett-Garg mixed state, the measured maximum value exceeds the classical maximum but is within the quantum bound; in the CHSH pure state the quantum and classical bounds are identical, and the measured value is within those bounds.

IV.2. Leggett-Garg Inequality

The Leggett-Garg quantity was measured according to the procedure given in III.3. Results for the $|0\rangle+|1\rangle$ state are given in Figure 6. As with the CHSH measurement, the signal seems to be suppressed for larger values of θ. However, in this case, θ means longer time delays and not longer pulses, so the contribution from incorrect pulse timings is less significant. On the other hand, the total running time for the trials with longer delays is more than 10 ms, which is a sizable fraction of the carbon T_2^*. This indicates that environmental interference may play a larger part in the large-θ trials.

The measured maximum values for each inequality are compared to the predicted classical and quantum values in Table I.

V. CONCLUSION

We have successfully simulated two Bell inequality violations in a liquid NMR system. Although simulating these violations does not prove that local realism must be abandoned, it does help in understanding experiments that actually demonstrate Bell inequality violations. These experiments have profound philosophical consequences.

If, in fact, Bell inequality violations are confirmed without any loopholes, then either information can travel faster than the speed of light, or quantum mechanics extends beyond a limit on measurements, and quantum uncertainty and entanglement are “real” in some sense. For example, Heisenberg’s uncertainty principle claims that if a particle’s position is measured precisely, its momentum cannot be measured. Bell inequality violations enable us to go one step further, to say that once a particle’s position is measured precisely, it no longer makes sense to talk about what would have happened if its momentum had been measured instead.

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