Violation of a Bell-like Inequality in Neutron Optical Experiments: Quantum contextuality

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Abstract. We report a single-neutron optical experiment to demonstrate the violation of a Bell-like inequality. Entanglement is achieved not between particles, but between the degrees of freedom, in this case, for a single-particle. The spin-1/2 property of neutrons are utilized. The total wave function of the neutron is described in a tensor product Hilbert space. A Bell-like inequality is derived not by a non-locality but by a contextuality. Joint measurements of the spinor and the path properties lead to the violation of a Bell-like inequality. Manipulation of the wavefunction in one Hilbert space influences the result of the measurement in the other Hilbert space. A discussion is given on the quantum contextuality and an entanglement-induced correlation in our experiment.

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1. Introduction

In a classic paper, Einstein, Podolsky, and Rosen (EPR) suggested the incompleteness of quantum theory by considering the reality given by the wave function of two physical quantities \(\hat{A}\). Their 'paradox' was moved forward to additional supplemented variables, towards a theory intending to reestablish a quantum mechanics with both causality and locality \[2\]. It was Bell who introduced an inequality to show the inconsistency of the hidden-variable theory and the statistical predictions of quantum theory \[3\]. His inequality was reformulated in various ways to adapt to real experimental tests of local hidden-variable theories. The most useful form may be so-called CHSH inequalities (Clauser-Horne-Shimony-Holt inequalities) \[4\]. Bell's inequalities together with the EPR-paradox have aroused considerable interests for many decades \[5, 6, 7\]. The contradiction inherent in such non-local phenomena with our common experience can be intuitively understood, because one usually considers the result of any specific measurement independent of what is to be measured at a distance. Within quantum terminology, this non-locality can be interpreted as a consequence of the correlation between commuting observables due to the different position where the measurements are done. Thus, a more general concept, i.e., contextuality, compared to non-locality can be introduced to describe other striking phenomena predicted by quantum theory \[8, 9, 10\]. Quantum contextuality is defined as follows: the result of a measurement of \(\hat{A}\) depends on another measurement on observable \(\hat{B}\), although these two observables commute with each other. It should be emphasized here that the property of locality is a special case of non-contextuality.

Except for the experiment with protons \[11\], most experimental tests of Bell’s inequalities have been performed with correlated photon pairs \[12, 13, 14, 15\]. In correlated photon experiments, two photons are emitted in a \(J=0 \rightarrow J=1 \rightarrow J=0\) atomic cascade or a parametric down-conversion. Thus, the state of the emitted photon pairs is described by a polarization entangled state. Since the wave function of each particle belongs to a different Hilbert space, an observable, e.g., the polarization of one photon, commutes with those for the other photon. Thus, no correlation between pairs is expected in general. Entanglement between pair photons, nevertheless, leads to remarkable correlations in polarization measurements.

Neutron optical experiments, based on interference of matter waves, have provided elegant demonstrations of the effects related to the fundamental aspects of quantum physics. In particular, neutron interferometer experiments have aroused affection for more than two decades \[16, 17, 18, 19\]. Among them, those with a polarized incident beam served as an ideal tool to investigate properties of a spin-1/2 system \[20\].

Here, we report an experiment of single-neutron interferometry to show the violation of a Bell-like inequality. In contrast of the conventional experiments with entangled particle pairs, the entanglement in our case is accomplished between different degrees of freedom of a single particle, i.e., we consider the entanglement between the spinor part and the spatial part of the wave function. Spin-1/2 particles, like neutrons, are
described in a tensor product Hilbert space, \( H = H_1 \otimes H_2 \) where \( H_1 \) and \( H_2 \) are disconnected Hilbert spaces corresponding to the spinor and the spatial wave function respectively. Observables of the spinor part commute with those of the spatial part, and this justifies the derivation of a Bell-like inequality equivalent to the rejection of the hypothesis of local realism [21]. The experiment consists of joint measurements of commuting observables of single neutrons in an appropriately prepared nonfactorisable state. A brief report of the experimental results has been published previously [22].

2. Theory

Most experimental tests of the violation of Bell’s inequalities have been made with correlated photon pairs. There, a source was used to emit entangled photon pairs in a Bell-state, for instance,

\[
|\Psi_{ab}\rangle = |H\rangle_a \otimes |V\rangle_b + |V\rangle_a \otimes |H\rangle_b, \tag{1}
\]

where \( |H\rangle \) and \( |V\rangle \) denote the horizontally and the vertically polarized states respectively. \( |\Psi_{ab}\rangle \) represents an entangled state, which shows a correlation and/or an anticorrelation. Here, CHSH inequalities are summarized as follows [23]:

\[
-2 \leq S \leq 2, \tag{2}
\]

with

\[
S = E\left(\vec{a}, \vec{b}\right) - E\left(\vec{a}, \vec{b}'\right) + E\left(\vec{a}', \vec{b}\right) + E\left(\vec{a}', \vec{b}'\right). \tag{3}
\]

where \( E\left(\vec{a}, \vec{b}\right) \) represents the expectation value of finding one photon \( a \) in polarization oriented to \( \vec{a} \) and the other \( b \) in polarization oriented to \( \vec{b} \). In real experiments, this polarization correlation coefficient is given by coincidence counts \( N \),

\[
E\left(\vec{a}, \vec{b}\right) = \frac{N_{++} \left(\vec{a}, \vec{b}\right) + N_{--} \left(\vec{a}, \vec{b}\right) - N_{+-} \left(\vec{a}, \vec{b}\right) - N_{-+} \left(\vec{a}, \vec{b}\right)}{N_{++} \left(\vec{a}, \vec{b}\right) + N_{--} \left(\vec{a}, \vec{b}\right) + N_{+-} \left(\vec{a}, \vec{b}\right) + N_{-+} \left(\vec{a}, \vec{b}\right)}. \tag{4}
\]

The signs of ”+” and ”−” denote the two outputs of the two-channel polarization analyzers for the parallel and the (orthogonal) perpendicular polarization.

Let us consider the principle of the experiment which demonstrates the violation of a Bell-like inequality in a single-neutron interferometry. Figure 1 shows the experimental setup. This setup is similar to that of a previous neutron interferometry for the spin superposition experiment [24]. In a polarized neutron interferometer experiment, the wave function of each neutron is described in a tensor product Hilbert space by the product of a spinor and a spatial wave function. This wave function represents the entanglement of the spinor part and the spatial part. The normalized total wave function \( |\Psi\rangle \) is given by

\[
|\Psi\rangle = \frac{1}{\sqrt{2}} \left( |\downarrow\rangle \otimes |I\rangle + |\uparrow\rangle \otimes |\Pi\rangle \right). \tag{5}
\]
Here, $|\uparrow\rangle$ and $|\downarrow\rangle$ denote the up- and down-spin states, and $|I\rangle$ and $|II\rangle$ the two beam paths in the interferometer. We introduce two operators projecting the spin part into orthogonal spin states, $\frac{1}{\sqrt{2}} (|\uparrow\rangle \pm e^{i\alpha} |\downarrow\rangle)$, which are given by

$$\hat{P}_s^{\alpha;\pm} = \frac{1}{2} (|\uparrow\rangle \pm e^{i\alpha} |\downarrow\rangle) \left(\langle\uparrow| \pm e^{-i\alpha} \langle\downarrow|\right).$$

(6)

In the same manner, two other projection operators for the path into orthogonal states, $\frac{1}{\sqrt{2}} (|I\rangle \pm e^{i\chi} |II\rangle)$ are defined as,

$$\hat{P}_p^{\chi;\pm} = \frac{1}{2} (|I\rangle \pm e^{i\chi} |II\rangle) \left(\langle I| \pm e^{-i\chi} \langle II|\right).$$

(7)

Here, parameters $\alpha$ and $\chi$ describe the spinor rotation and the phase shift in the experiments.

The expectation value for a joint measurement of the spin state $\frac{1}{\sqrt{2}} (|\uparrow\rangle + e^{i\alpha} |\downarrow\rangle)$ and the path $\frac{1}{\sqrt{2}} (|I\rangle + e^{i\chi} |II\rangle)$ is calculated to be

$$E'(\alpha, \chi) = \langle \Psi | \hat{P}_s^{\alpha} \cdot \hat{P}_p^{\chi} |\Psi\rangle$$

$$= \langle \Psi | \left[(+1) \cdot \hat{P}_s^{\alpha;+1} + (-1) \cdot \hat{P}_s^{\alpha;-1}\right]$$

$$\times \left[(+1) \cdot \hat{P}_p^{\chi;+1} + (-1) \cdot \hat{P}_p^{\chi;-1}\right] |\Psi\rangle,$$

(8)

where $\hat{P}_s^{\alpha}$ and $\hat{P}_p^{\chi}$ are observables for the spin and the path, respectively, and are decomposed by the projection operators given by Eqs. (6) and (7). This expectation value is analogous to that of a joint measurement, $E \left(a_j, b_k\right)$, for correlated-photon-pair experiments [23]. It should be emphasized here that the observables $\hat{P}_s$ and $\hat{P}_p$ operate on the different Hilbert space, then they commuting with each other.

A Bell-like inequality for the single-neutron interferometry uses the quantity $S'$ which is expressed with expectation values $E'(\alpha, \chi)$ [27]:

$$-2 \leq S' \leq 2,$$

(9)

with

$$S' = E'(\alpha_1, \chi_1) - E'(\alpha_2, \chi_2) + E'(\alpha_3, \chi_3) + E'(\alpha_4, \chi_4).$$

(10)

In two-photon correlation experiments, the polarization correlation coefficient is practically given with coincidence counts $N$. We consider here in more detail of the practical deviations of the expectation value $E'(\alpha, \chi)$. The operators $\hat{P}_s^{\alpha;+1}$ and $\hat{P}_p^{\chi;+1}$ can be realized with the spin-rotator for $\alpha$ and the phase shifter for $\chi$. In addition, since $\hat{P}_s^{\alpha;-1} = \hat{P}_s^{\alpha+\pi;+1}$ and $\hat{P}_p^{\chi;-1} = \hat{P}_p^{\chi+\pi;+1}$, the operators $\hat{P}_s^{\alpha;-1}$ and $\hat{P}_p^{\chi;-1}$ can also be realized with the appropriate rotation of the spin-rotator $\alpha + \pi$ and position of the phase shifter $\chi + \pi$. Therefore, the expectation value $E'(\alpha, \chi)$ will be practically given by
$$E'(\alpha, \chi) = \frac{N'_{++}(\alpha, \chi) + N'_{--}(\alpha, \chi) - N'_{+-}(\alpha, \chi) - N'_{-+}(\alpha, \chi)}{N'_{++}(\alpha, \chi) + N'_{--}(\alpha, \chi) + N'_{+-}(\alpha, \chi) + N'_{-+}(\alpha, \chi)}$$

$$= \frac{N'_{++}(\alpha, \chi) + N'_{++}(\alpha + \pi, \chi + \pi) - N'_{--}(\alpha, \chi + \pi) - N'_{++}(\alpha + \pi, \chi)}{N'_{++}(\alpha, \chi) + N'_{++}(\alpha + \pi, \chi + \pi) + N'_{++}(\alpha, \chi + \pi) + N'_{++}(\alpha + \pi, \chi)},$$

(11)

where $N'_{++}(\alpha_j, \chi_k)$ denotes the count rate with the spin-rotation of $\alpha_j$ and the phase shift of $\chi_k$, which is described by

$$N'_{++}(\alpha_j, \chi_k) = \langle \Psi | \hat{P}_{s;+}^{\alpha_j+1} \cdot \hat{P}_{p;+}^{\chi_k+1} | \Psi \rangle.$$  

(12)

Relations between the coincidence counts, $N$, in the two-photon correlation experiments and the count rates, $N'$, in the single-neutron interferometer experiment are summarized in the following:

$$N_{++}(\vec{a}, \vec{b}) : N'_{++}(\alpha, \chi)$$

$$N_{--}(\vec{a}, \vec{b}) : N'_{--}(\alpha, \chi) = N'_{++}(\alpha + \pi, \chi + \pi)$$

$$N_{+-}(\vec{a}, \vec{b}) : N'_{+-}(\alpha, \chi) = N'_{++}(\alpha, \chi + \pi)$$

$$N_{-+}(\vec{a}, \vec{b}) : N'_{-+}(\alpha, \chi) = N'_{++}(\alpha + \pi, \chi).$$

(13)

Equations (13) account for the possibility to measure the count rates $N'$ not simultaneously with different detectors but successively with one detector. The appropriate observables are tuned by the spin-rotator and the phase shifter. In this case, a fair-sampling hypothesis is required to justify obtaining expectation values from such successive measurements.

Quantum theory predicts a sinusoidal behaviour for the count rate $N'_{++}^{qm}(\alpha, \chi) = \frac{1}{2} \{1 + \cos(\alpha + \chi)\}$. The same behaviour is also derived for the expectation value $E'(\alpha, \chi) = \cos(\alpha + \chi)$. These functions will lead to a violation of the Bell-like inequality for various sets of polarization analysis and phase shift. The maximum violation is expected, for instance, for the following set: $\alpha_1 = \pi/2$, $\alpha_2 = 0$, $\chi_1 = -\pi/4$, and $\chi_2 = \pi/4$ to show $S' = 2\sqrt{2} = 2.82 > 2$.

So far we have described the experiment in terms of perfect implementation. In the actual experiment, however, perfect sinusoidal dependence of $N'$ cannot be established due to unavoidable component misalignments, imperfect quality of polarization/interference, etc., which is characterized by contrasts of the oscillations. When the visibility of the oscillation due to the spin-rotation and/or the phase shift is reduced, it is expected that the theoretical predictions for $N'$ and $E'$ reduce proportionally, thus $S'$ getting smaller by the same factor. The experiment to demonstrate the violation of the Bell-like inequality requires a final visibility higher than $\sqrt{2}/2 = 70.7\%$. The interfering H-beam does not satisfy this condition in practical
neutron interferometer experiments. Thus, our experiment utilizes only the O-beam, which, in principle, has 100% visibility. The count rates \( N'_{\pm}(\alpha, \chi) \) are measured not simultaneously but successively with appropriate spin-rotations and phase shifts.

3. Experiments

Our experiment consists of three stages: preparation, manipulation, and detection. The preparation was achieved by the use of a spin-turner after the polarized beam was split into two paths, producing a Bell state, \( |\Psi\rangle = \frac{1}{\sqrt{2}} (|\rightarrow\rangle \otimes |I\rangle + |\leftarrow\rangle \otimes |II\rangle) \). In the manipulation, the two parameters of \( \alpha \) and \( \chi \) were adjusted. And finally, the neutrons with certain properties were detected. We utilized a polarization analysis on the O-beam to obtain correlation coefficients.

Figure 1. Schematic view of the experimental setup to demonstrate the violation of a Bell-like inequality in single-neutron interferometry. The experiment consists of three stages: a preparation of the entangled state \( |\Psi\rangle = \frac{1}{\sqrt{2}} (|\rightarrow\rangle \otimes |I\rangle + |\leftarrow\rangle \otimes |II\rangle) \) with the use of the spin-turner, a manipulation of the two parameters, a phase shift of \( \chi \) and the spinor rotation angle of \( \alpha \) together with a Heusler-analyser, and a detection.

The experiment was carried out at the perfect crystal interferometer beam line S18 at the high flux reactor of the Institute Laue Langevin (ILL) [25]. A schematic view of the experimental setup is given in Fig. 1. The neutron beam was monochromatized to have a mean wave length of \( \lambda_0 = 1.92\text{Å} \) by the use of a Si perfect crystal monochromator. The incident beam was polarized vertically by magnetic-prism refractions, then entering a triple-Laue (LLL) interferometer. This interferometer was adjusted to give a 220 reflection. A parallel-sided Si plate was used as a phase shifter (varying \( \chi \)). A pair of water-cooled Helmholtz coils produced a fairly uniform magnetic guide field, \( B_0\hat{z} \), around the interferometer. A magnetically saturated Heusler crystal together with
a rectangular spin rotator (adjusting $\alpha$) and a spin flipper, if necessary, enabled the selection of neutrons with certain polarization directions.

![Diagram](image)

**Figure 2.** Interference oscillations for two-level systems: (a) for a spatial Hilbert-space and (b) for a polarization Hilbert-space. The contrasts over 91% for (a) and about 95% for (b) were achieved. This confirmed the capability of our manipulation for the path and the spinor subsystems.

A crucial optical element in our preparation is a spin turner, which turns the incident spinor $|\uparrow\rangle$ to $|\rightarrow\rangle$ for one beam and to $|\leftarrow\rangle$ for the other. For this procedure, we utilized a soft-magnetic Mu-metal sheet [26], which gives considerably high permeability induced by pretty weak magnetic field. A sheet of 0.5mm thick in an oval ring form was used and two DC-coils were applied to magnetize this soft-magnetic sheet.

The important parameters for the manipulation are the relative phase, $\chi$, between the two beams and the spinor rotation angle, $\alpha$. To test the capability of our apparatus, we have measured interference oscillations for two two-level systems in the interferometer: one for a spatial system, i.e., controlling the path, and the other for a spinor system, i.e., controlling the spin. Typical oscillations are shown in Fig. 2. One observes sinusoidal oscillations when varying the parameters $\chi$ for (a) and $\alpha$ for (b). Sufficiently high contrast values were achieved, which confirmed the capability of our apparatus for manipulating two subsystems, i.e., the path and the spin, of neutrons in the interferometer.

A maximum violation of the Bell-like inequality is expected for setting the spinor rotation angle $\alpha$ at $0$, $\pi/2$, $\pi$, and $3\pi/2$. Typical intensity modulations, obtained by varying the phase shift $\chi$, are shown in Fig. 3. Contrasts evidently fell down from those shown in Fig. 2 mainly due to dephasing/depolarization at the Mu-metal spin-turner. Its gradual reduction by increasing $\alpha$ is attributed to slight depolarization by the spinor-rotator and the $\pi$-spin-flipper. We, however, achieved to obtain enough high contrasts, more than 70.7%, to accomplish the experiment. Since the Mu-metal spin-turner induces additional relative phase shift between two-beams in the interferometer,
Figure 3. Typical interference oscillations with spinor rotation angle $\alpha = 0$, $\pi/2$, $\pi$, and $3\pi/2$. Contrasts of 76% for one and about 73% for the other three were achieved. Expectation values, $E_{\text{obs}}$, were derived from the intensities of appropriate $\chi$ [on the lines (a) $\chi=0.79\pi$ and (a') $\chi=1.79\pi$, or (b) $\chi=1.29\pi$ and (b') $\chi=0.29\pi$], where a maximum violation of the Bell-like inequality is expected. These values exhibited the final $S'$ value of $2.051 \pm 0.019 > 2$: clear violation of the Bell-like inequality.

All interference oscillations are shifted by about $\pi$ in this figure. We took this shift into account in determining appropriate $\chi$-positions to show the maximum violation.

After fitting to sinusoidal dependence by the least squares method, the expectation values $E_{\text{obs}}$ were determined using Eq. (11). Typical statistical error of $E_{\text{obs}}$ was 0.01, obtained from curves of single measurement. We repeated the same measurements at least 16 times to reduce statistical errors. The final value $E_{\text{obs}}$ and its error were evaluated by weighted average of all measurements. So, the final errors are the sum of systematic and statistical errors. (Main reason for systematic error was due to phase instability, random drift of phase, during the measurement.) We obtained $E_{\text{obs}}(0, 0.79\pi)$, to be $0.542 \pm 0.007$ from the intensities of $N'(0, 0.79\pi)$, $N'(\pi, 0.79\pi)$, $N'(0, 1.79\pi)$, and $N'(\pi, 1.79\pi)$. In the same manner, we obtained $E_{\text{obs}}(0, 1.29\pi) = 0.4882 \pm 0.012$, $E_{\text{obs}}(0.5\pi, 0.79\pi) = -0.538 \pm 0.006$, and $E_{\text{obs}}(0.5\pi, 1.29\pi) = 0.438 \pm 0.012$. In evaluating the Bell-like inequality, $S'$ was calculated to be

$$S' \equiv E'(\alpha_1, \chi_1) + E'(\alpha_1, \chi_2) - E'(\alpha_2, \chi_1) + E'(\alpha_2, \chi_2)$$

$$= 2.051 \pm 0.019 > 2.$$  \hspace{1cm} (14)

for $\alpha_1, \alpha_2=0, 0.50\pi$, and $\chi_1, \chi_2=0.79\pi, 1.29\pi$, respectively. This clearly shows a violation.
of the Bell-like inequality, which results from the quantum contextuality.

4. Discussions

The results given above were obtained by using a neutron detector of more than 99% efficiency [27]. In this case, however, a fair-sampling hypothesis is still required, because of losses in the interferometer—the second plate of the interferometer is not a mirror but a beam-splitter—in addition to the fact that the count rates were obtained successively one after another. It is possible to introduce the term quantum contextuality in the discussion of our experiments. The observable for the path and the spin belong to different Hilbert spaces in our experiments, therefore they commute with each other. Nevertheless, the expectation value for a joint measurement, \( E'(\alpha, \chi) \) shows correlation between two observables due to the entanglement between two degrees of freedom of a single-particle. It is worth noting here that entanglement is not limited to different particles but generally applicable to different subsystems, thus a correlation between variables in single particles being also expected. General arguments on the entanglement-induced correlation can be found in the literature [28, 29].

We can interpret the expectation value \( E'(\alpha, \chi) \) in terms of beam polarizations as frequently used in neutron optics: ‘conditional’ polarization of ‘path’ and ‘spin’ polarizations. These polarizations vary from \(-1\) to \(+1\). The maximum violation of the Bell-like inequality occurs for a set of four polarization measurements, three of them resulting in \(+\sqrt{2}/2\) and the other in \(-\sqrt{2}/2\). The value \( E' \) can not be factorized as

\[
E'(\alpha, \chi) = \cos (\alpha + \chi) \\
\neq \cos \alpha \cdot \cos \chi = P^s(\alpha) \cdot P^p(\chi),
\]

although \( \hat{P}^{s,\pm}_{\alpha} \) and \( \hat{P}^{p,\pm}_{\chi} \) commute with each other: a non-factorizable expectation value \( E' \) for the conditional polarization by \( \alpha \) for the spin and \( \chi \) for the path. In other words, results of the measurements for the spin- and the path-polarization are correlated due to the fact that the subsystems in single neutron are entangled. Such a correlations involved in our experiments can be used for another realization of delayed-choice experiment and a new technique of manipulation, e.g., non-contact control.

5. Conclusions

We report an interferometric experiment with a single spin-1/2 neutron which demonstrates the violation of a Bell-like inequality. The wave function of the neutron is described within a tensor product of Hilbert spaces, one for the spinor part and the other for the spatial part of the wave function. Appropriate combinations of spin-rotation and phase shift lead to the violation of a Bell-like inequality not with correlated particles but with measurements for single neutrons. A correlation between subsystems in single particles is induced by entanglement.
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