Noncyclic Pancharatnam phase for mixed state SU(2) evolution in neutron polarimetry

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We have measured the Pancharatnam relative phase for spin-1/2 states. In a neutron polarimetry experiment the minima and maxima of intensity modulations, giving the Pancharatnam phase, were determined. We also considered general SU(2) evolution for mixed states. The results are in good agreement with theory.

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I. INTRODUCTION

In recent years much attention has been paid to the concept of geometric phase. Since its discovery by Berry \cite{Berry1984} the subject was widely expanded and subdued to several generalizations \cite{Thacker1986}, e.g. non adiabatic \cite{Thacker1986} and non-cyclic \cite{Thacker1986} evolutions as well as the off-diagonal case \cite{Thacker1986}. Ever since, a great variety of experimental confirmations of the Berry phase and its peculiar properties have been accomplished (see e.g. \cite{Marino2005, Das2003, Zagoskin2000, Du2004, Ericsson2005}). In 1956 Pancharatnam defined $\phi = \arg \langle \psi_0 | \psi \rangle$ as the phase acquired during an entirely arbitrary evolution of a wave-function \cite{Pancharatnam1956}. Provided the evolution takes place under condition of parallel transport, $\phi$ can be identified with the noncyclic geometric phase. Quite recently, also a concept of mixed state phase was developed by Sjöqvist et al. \cite{Sjoqvist2000} due to its importance in quantum computation. The theoretical predictions have been tested by Du et al. \cite{Du2004} and Ericsson et al. \cite{Ericsson2005} using NMR and single-photon interferometry, respectively. In this letter, we report a neutron polarimetry experiment for measuring the Pancharatnam relative phase of a spinor subdued to an arbitrary SU(2) evolution, implementing the method described by Wagh and Rakhecha in \cite{Wagh1990}. We test its extension to the mixed state case put forward by Larsson and Sjöqvist \cite{Larsson2001}.

II. THE PURE STATE CASE

We consider the experimental setup shown in Fig. 1. A monochromatized neutron beam, polarized along the $+z$ direction experiences a $\pi/2$ flip about the $x$-axis, therefore being denoted as a superposition of the orthogonal states $|\pm z\rangle$. The beam travels in an overall guide field $B_z$ of the length $L$, which is chosen to be parallel to the $+z$ direction. Under the influence of $B_z$ the polarization vector rotates through an angle $\eta$ determined by the distance $L$. The two orthogonal components $|\pm z\rangle$ of the rotated superposition state acquire opposite phase undergoing the SU(2) transformation $U_0$, denoted by the matrix

$$U_0(\xi, \delta, \zeta) = \begin{pmatrix} e^{i\delta} \cos \xi & -e^{-i\delta} \sin \xi \\ e^{i\xi} \sin \xi & e^{-i\delta} \cos \xi \end{pmatrix}. \quad (1)$$

In neutron polarimetry the unitary, unimodular operator $\hat{U}(\vec{a})$ is used for description of spin rotations (transformations) carried out within magnetic fields. By comparison of Eq. (1) to the matrix representation of $\hat{U}(\vec{a})$, with

$$\hat{U}(\vec{a}) = \exp \left( -i \frac{\vec{\sigma} \cdot \vec{a}}{2} \right)$$

$$= \hat{1} \cos \frac{a}{2} - i \left( \hat{\sigma_x} \frac{a_x}{2} + \hat{\sigma_y} \frac{a_y}{2} + \hat{\sigma_z} \frac{a_z}{2} \right) \sin \frac{a}{2}, \quad (2)$$

one is lead to sets $(\xi, \delta, \zeta)$ of SU(2) parameters. $\vec{a}$ points to the direction of the magnetic field constituting the rotation axis and $|\vec{a}| = a$ denotes the rotation angle. $\vec{\sigma}$ is the Pauli vector operator. The resulting beam passes a distance $L'$ along the guide field $B_z$, its polarization rotating through the associated angle $2n\pi - \eta (n = 1, 2, ...)$.
\[ L_0 = L + L' \] is set in such a way that the accumulated rotation angle within \( B_z \) equals an integer multiple of \( 2\pi \). Finally, a \( -\pi/2 \) flip around the \( x \)-axis is applied and the output intensity, calculated as

\[ I = \cos^2 \xi \cos^2 \delta + \sin^2 \xi \sin^2 (\zeta + \eta) \] (3)

for the pure state case, is measured. The phase shift \( \eta \), implemented by variation of the distances \( L \) and \( L' \) at constant \( L_0 \) causes intensity modulations, yielding the extreme values

\[ I_{\text{min}} = \cos^2 \xi \cos^2 \delta, \]
\[ I_{\text{max}} = \cos^2 \xi \cos^2 \delta + \sin^2 \xi. \] (4) (5)

In our case, the Pancharatnam phase \( \phi \) is given by substituting \(|\psi_0\rangle\) by \(|+z\rangle\) and \(|\psi\rangle\) by \(|U_0| + z\rangle\). The relative phase shift between \(|+z\rangle\) and \(|U_0| + z\rangle\), \( \phi = \arg \langle z|U_0| + z\rangle = \delta + \arg \cos \xi \) for the pure state case, is therefore computed from

\[ \phi = \arccos \sqrt{\frac{I_{\text{min}}}{1 - I_{\text{max}} + I_{\text{min}}}}. \] (6)

### III. THE MIXED STATE CASE

More general, a neutron beam passing the setup explained above at any arbitrary degree of polarization \( r \) along the positive \( z \)-axis is described by the density operator

\[ \hat{\rho} = \frac{1}{2} (\hat{1} + r \hat{\sigma}_z), \] (7)

with the Pauli spin operator \( \hat{\sigma}_z \) and \( 0 \leq r \leq 1 \). The measured intensity for this mixed state is given by

\[ I^\rho = \frac{1 - r}{2} + r I, \] (8)

which obviously reduces to Eq. (3) for \( r = 1 \). The relative mixed state phase \( \Phi \) is

\[ \Phi = \arctan[r \tan(\delta + \arg \cos \xi)]. \] (9)

With the associated extreme values of Eq. (5) for \( r \geq 0 \),

\[ I^\rho_{\text{min}} = \frac{1 - r}{2} + r \cos^2 \xi \cos^2 \delta \]
\[ I^\rho_{\text{max}} = \frac{1 - r}{2} + r(\cos^2 \xi \cos^2 \delta + \sin^2 \xi), \] (10) (11)

one obtains the following expression for the mixed state relative phase \( \Phi \):

\[ \Phi = \arccos \sqrt{\frac{I^\rho_{\text{min}} - 1/2(1-r)}{r^2[1/2(1+r) - I^\rho_{\text{max}}] + I^\rho_{\text{min}} - 1/2(1-r)}}. \] (12)

This formula is consistent with the pure state case since for \( r = 1 \) it reduces to Eq. (4). The density operator formalism is subject to an ambiguity, in a sense that certain inherently distinct physical situations are described by identical density matrices. This is often referred to as 'decomposition freedom' (see e.g. [18]). Moreover, it is not apparent from Eq. (17) by what means some mixed state of the system should be produced. Considering this, we introduced a \( \pi \) flip in front of the actual setup, resulting in a beam polarized in the \( -z \) direction. The intensities \( I_{\text{off}} \) and \( I_{\text{on}} \), corresponding to 'spin flipper off' and 'spin flipper on', respectively, were measured for equal time intervals. A density matrix was calculated from a weighted sum of \( I_{\text{off}} \) and \( I_{\text{on}} \) referring to a certain degree of polarization \( r \geq 0 \) and is therefore equivalent to the associated mixed state. Since a real polarizer does not work perfectly, it is important to note that the incident neutron beam can already be considered to be in a mixed state, as it was done in this work. For many experiments, in contrast, it is sufficient to assume the incident beam to be purely polarized in some arbitrarily chosen direction.

### IV. EXPERIMENT

The experiment was carried out at the tangential beam port of the 250 kW TRIGA research reactor of the Atomic Institute of the Austrian Universities, Vienna. The neutron beam of mean wavelength \( \lambda = 1.999 \text{ Å} \), incident from a pyrolytic graphite monochromator, was polarized along the \( +z \) direction by reflection from a bent Co-Ti supermirror array. All spin rotations were implemented by Larmor precessions about the magnetic field axes of DC coils made of anodized aluminium wire wound on frames with rectangular profile. After passing the DC \( \pi \) flipper the beam encounters the first \( \pi/2 \) spin turner creating a superposition of the orthogonal states \(|\pm z\rangle\). The polarization vector precesses in the \( xy \)-plane through the angle \( \eta \) around the \( +z \) direction in the guide field \( B_z \) and length \( L \) at an angular frequency \( \omega = \frac{2\pi}{\hbar} B_z \).
guide field of length $L_0$ was realized by two rectangular coils of 150 cm length along the beam trajectory and a width of 12 cm. They were arranged in Helmholtz geometry to provide for optimal homogeneity. The combination of the guide field $B_z$ measured by a Hall probe (= 5.893 ± 0.022 G) and the distance 4 $L_0$ (about 46 cm) was chosen in such a way that more than one period ($\eta > 2\pi$) of intensity oscillations could be scanned for its extreme values. The subsequent SU(2) transformation $U_0(\xi, \delta, \zeta)$ was carried out by two coils with mutually orthogonal orientation wound on the same frame. Along the distance $L'$ from the SU(2) coils to the second spin turner the polarization vector precesses by an angle $2\pi - \eta$ about the guide field $B_z$ before being turned through $-\pi/2$ about the $x$-axis, analyzed in the $+z$ direction by a second supermirror array and finally counted by a $^3$He detector. The variation of the phase shift $\eta$ is implemented by physical translation of the two $\pi/2$ spin turners at constant distance $L_0 = L + L'$. This can be done conveniently by steps of some mm, exhibiting the intensity oscillations evoked by the phase shift $\eta$.

Here, we present the results for two settings of SU(2) coil currents. For each set of transformation parameters $(\xi, \delta, \zeta)$, three minima and maxima of $I_{\text{off}}$ and $I_{\text{on}}$ were measured in one scan. Given uncertainties contain both systematic and statistical errors. The first example is a rotation as depicted schematically in Fig. 2A. The associated SU(2) parameter set is $(\xi^{(A)}, \delta^{(A)}, \zeta^{(A)}) \rightarrow (1.71, 0.38, -1.46)$ rad. By application of Eq. (12) one obtains the theoretical result $\Phi_{\text{th}}^{(A)} = 0.37$ rad, whereas the value computed from the measured data using Eq. (12) is $\Phi_{\text{m}}^{(A)} = 0.38 \pm 0.08$ rad at initial polarization $r^{(A)}_0 = 0.976 \pm 0.004$. The measured intensities $I_{\text{off}}, I_{\text{on}}$ and the calculated mixed state intensities for three different degrees of polarization are shown in Fig. 2A and B, respectively. The second example is depicted in Fig. 2B, being described by parameters $(\xi^{(B)}, \delta^{(B)}, \zeta^{(B)}) \rightarrow (1.06, 0.17, -1.40)$ rad. For this set the theoretical prediction is $\Phi_{\text{th}}^{(B)} = 0.17$ rad. The experimental result is $\Phi_{\text{m}}^{(B)} = 0.16 \pm 0.06$ rad at initial polarization $r^{(B)}_0 = 0.981 \pm 0.005$. Measured and calculated intensities are shown in Fig. 2A and B. For the density matrices derived from the experimental data the results are $\Phi_{0.8}^{(A)} = 0.35 \pm 0.06$ (0.31) rad, $\Phi_{0.6}^{(A)} = 0.21 \pm 0.06$ (0.24) rad, $\Phi_{0.3}^{(A)} = 0.05 \pm 0.07$ (0.12) rad for the transformation $(\xi^{(A)}, \delta^{(A)}, \zeta^{(A)})$ and $\Phi_{0.8}^{(B)} = 0.12 \pm 0.06$ (0.14) rad, $\Phi_{0.6}^{(B)} = 0.10 \pm 0.07$ (0.10) rad, $\Phi_{0.3}^{(B)} = 0.02 \pm 0.08$ (0.05) rad for $(\xi^{(B)}, \delta^{(B)}, \zeta^{(B)})$. The values in parenthesis are the corresponding theoretical predictions for $\Phi$ calculated from Eq. (12).
that for a certain angle $\theta$ beam is governed by the Bragg condition $2d \sin \theta = n\lambda$, where $d$ is the lattice spacing, $\theta$ the angle, $n$ an integer, and $\lambda$ the wavelength of the incident radiation. This can be explained as an effect of second order neutron interference, as slight irregularities in height as can be seen in the graphs.

The extreme values of the intensity modulations show slight irregularities in height as can be seen in the graphs. This can be explained as an effect of second order neutrons (wavelength $\lambda/2$). The monochromatization of the beam is governed by the Bragg condition $2d \sin \theta_B = n\lambda$, that is for a certain angle $\theta_B$ - is fulfilled for $n= 1, 2, ...$. Consequently, the beam used for the experiment is contaminated by a percentage of neutrons with only half the intended wavelength. In a time of flight (TOF) measurement, this percentage was found to be $\lesssim 7.2$ % of the overall intensity. Neutrons that travel at double velocity spend only half the time in magnetic fields along the beam trajectory. Therefore, their spin rotates through only half the originally intended angles, showing a behavior rather different from the first order intensity. To compute the relative phase, values for $I_{\text{max}}$ and $I_{\text{min}}$ were determined from a least-squares fitting model (also shown in Fig. 4 and Fig. 6), taking into account the second order neutrons. The careful reader will point out that randomness is missing in the mixing procedure described above: the relative frequencies for finding the system in either one of the pure states $|+z\rangle$ or $|-z\rangle$ are not only well known, but even determined by the experimenter. As a matter of fact, the actual system, the neutron beam, is at no time of the experiment in one of the mixed states associated with $r=0.8, 0.6$ or $0.3$. We are aware of the fact that the procedure carried out does by no means constitute a general mixing method, but represents a special approach within the wide scope of possible and accepted techniques for mixed state preparation. Nevertheless, the density matrices are generated by using the measured data resulting from the conducted experiments, fulfilling the predictions developed by Larsson and Sjöqvist [17].

A neutron optical experiment showing the $r$ dependence of the phase by application of some other preparation method will be carried out in the future.

The obtained experimental results are in good agreement with theoretical predictions for the relative mixed state phase, although systematic errors occur due to inherent difficulties of the experiment. Even though the guide field was constructed carefully, some inhomogeneity ($\sim 0.4\%$) along its length cannot be avoided completely, accumulating an error of $\sim 5^\circ$ in the angle $\eta$ along the distance $4L_0$. Furthermore, it was difficult to compute values for the readjustment of $4L_0$ after a change of SU(2) coil currents. Consequently, the correct distance between the spin turners was tuned by its variation at minimum intensity relative position of spin turners and SU(2) coils, thereby exhibiting the maximum of visibility. Another point is that the two $\pi/2$ spin turners were situated within the guide field. Therefore they did not exactly carry out the designated rotations of the polarization vector to the $-y$ direction and back to the $+z$ direction. These inaccuracies are intrinsic to this experiment and can hardly be avoided at considerable effort. Further discussions gave rise to interesting ideas for possible improvements of the experimental setup concerning accuracy and robustness. At present, they are tested and will be described in a forthcoming paper [19].

V. DISCUSSION

The relative phases of the intensity modulations show slight irregularities in height as can be seen in the graphs. This can be explained as an effect of second order neutrons (wavelength $\lambda/2$). The monochromatization of the beam is governed by the Bragg condition $2d \sin \theta_B = n\lambda$, that is for a certain angle $\theta_B$ is fulfilled for $n= 1, 2, ...$. Consequently, the beam used for the experiment is contaminated by a percentage of neutrons with only half the intended wavelength. In a time of flight (TOF) measurement, this percentage was found to be $\lesssim 7.2$ % of the overall intensity. Neutrons that travel at double velocity spend only half the time in magnetic fields along the beam trajectory. Therefore, their spin rotates through only half the originally intended angles, showing a behavior rather different from the first order intensity. To compute the relative phase, values for $I_{\text{max}}$ and $I_{\text{min}}$ were determined from a least-squares fitting model (also shown in Fig. 4 and Fig. 6), taking into account the second order neutrons. The careful reader will point out that randomness is missing in the mixing procedure described above: the relative frequencies for finding the system in either one of the pure states $|+z\rangle$ or $|-z\rangle$ are not only well known, but even determined by the experimenter. As a matter of fact, the actual system, the neutron beam, is at no time of the experiment in one of the mixed states associated with $r=0.8, 0.6$ or $0.3$. We are aware of the fact that the procedure carried out does by no means constitute a general mixing method, but represents a special approach within the wide scope of possible and accepted techniques for mixed state preparation. Nevertheless, the density matrices are generated by using the measured data resulting from the conducted experiments, fulfilling the predictions developed by Larsson and Sjöqvist [17].

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VI. CONCLUSION

To summarize, we have measured the Pancharatnam relative phase for the mixed state case in a neutron polarization experiment. The dependence of the phase of the degree of polarization was indicated by calculation of weighted sums of the density matrices corresponding to the measured intensities. The experimental data is in good agreement with theory. Deviations of the predicted behavior were explained to arise due to contamination of the beam by second order neutrons.

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