Reconstruction of the spin state

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I. INTRODUCTION

Quantum mechanics of 1/2 spin particles serves often as an illustrating example for many quantum considerations in standard textbooks of quantum theory. The importance of this model is enhanced by the fact that such states represent the smallest amount of quantum information – quantum bits (q-bits). Besides theoretically valuable “Gedanken” experiments, the spin 1/2 particles such as electrons, neutrons or polarization states of light quanta are convenient for feasible experiments in matter wave and quantum optics. They play crucial role in many sophisticated schemes involving entanglement, Bell state analysis or teleportation. Several approaches for measurement and estimation of spin states have been considered recently. In this Brief Report, the maximum likelihood (MaxLik) estimation of 1/2 spin state will be formulated as an illustrating example of more general treatment. The given formulation shows a tight relation between quantum and statistical theories. Synthesis of many independent and nonequivalent ideal detections of Stern–Gerlach (SG) type will be interpreted as a new generalized measurement, output of which the quantum state is. This consideration will be used as a basic tool for further investigation in depolarization measurements, neutron and light interferometry and quantum state reconstruction.

Basic properties of spin 1/2 quantum systems will be briefly reviewed. A pure state (projector) may be represented by the expression

$$|a\rangle\langle a| = \frac{1}{2}(1 + a_i\sigma_i),$$  \hspace{1cm} (1)

where \(a = (a_1, a_2, a_3)\) is the three-dimensional normalized vector, \(\sigma_i, i = 1, 2, 3\) represent the Pauli matrices and the summation convention for repeated indices is used. Since

$$\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k,$$

the scalar product of two projectors is given as

$$|a|b\rangle = \frac{1}{2}(1 + a_ib_i).$$

General state described by a density matrix may be parameterized by

$$\hat{\rho} = p_+|a\rangle\langle a| + p_-|-a\rangle\langle -a|$$  \hspace{1cm} (2)

$$\frac{1}{2} + \frac{1}{2}\sigma_i(a_+ - a_-),$$  \hspace{1cm} (3)

where \(p_+ + p_- = 1\) and the states \(|a\rangle, |-a\rangle\) denote a general orthogonal basis. Spin state may be alternatively described by a polarization vector

$$r_i = \langle \sigma_i \rangle = a_i(p_+ - p_-),$$  \hspace{1cm} (4)

where the brackets \(\langle \rangle\) denote an expectation value. Hence the polarization \(r_i\) completely determines the state of quantum system. Degree of polarization may be introduced as

$$|r|^2 \leq 1$$

and \(|r|^2 = 0\) for completely unpolarized (mixed) state and \(|r|^2 = 1\) for completely polarized (pure) states.

The polarization or spin may be measured by projecting the state into the given directions of SG apparatus \(\pm a\). Closure relation and operator representation of such a device simply read

$$|a\rangle\langle a| + |-a\rangle\langle -a| = \hat{1},$$  \hspace{1cm} (5)

$$\hat{A} = \frac{1}{2}\left[|a\rangle\langle a| - |-a\rangle\langle -a|\right].$$  \hspace{1cm} (6)

Assuming for the sake of simplicity always the same total number of particles \(N\), the number of particles with the spin “up” and “down” estimates projections of the polarization vector according to the relations

$$n_\pm = Np(\pm a) = \frac{1}{2}N(\pm ra).$$  \hspace{1cm} (7)

Since this may be done for three orthogonal directions of coordinate axes \(x_i, i = 1, 2, 3\), the polarization may be found by eliminating the total number of particles \(N\)
Each polarization component is determined separately. This represent a correct solution, provided that resulting polarization is inside the Poincaré sphere \(|r|^2 \leq 1\) only. This example has been used for motivation of general analysis of quantum state reconstruction in Ref. [7]. As demonstrated, the “states” outside the Poincaré sphere violate the positive semidefiniteness of quantum states yielding improper quantum description of noises. Similar problems appear in the case when more than three projections are used. Some results of SG projections might be interpreted as a novel measurement of quantum state. This example has been used for motivation of general analysis of quantum state reconstruction in Ref. [7].

This is manifested in quantum theory, since various SG apparatus may not commute for different orientations \(a^i\). Such measurements, even if done with equal number of particles, determine various “faces” of the spin system. Such measurements are not equivalent, since they are observing various fluctuations and noises involved. Various SG measurements are used. Some results of SG projections might be interpreted as a novel measurement of quantum state. This procedure must predict an unknown state and simultaneously take into account data fluctuations. This indicates the nonlinearities of an algorithm. MaxLik estimation does this job and fits the data to a quantum state. Besides this, it is the only procedure, which provides the same structure as generalized measurement \([8]\). Henceforth, synthesis of incompatible measurements may be interpreted as a novel measurement of quantum state. This will be demonstrated in the following section.

II. SPIN ESTIMATION

Provided that source supplies 1/2 spin particles prepared in the same mixed state, an ideal lossless SG measurement performed repeatedly on the system of \(N\) particles will be assumed. The setting of SG apparatus may change. Provided that detection has been done with \(M\) different settings, \(N \times M\) particles have been used altogether and an unknown quantum state should be found. The results of the measurement may be characterized by settings of the SG apparatus \(\pm a^i\) and by the relative frequencies of the outcomes \(1/2(1 \pm X_j) = n_{j, \pm}/N\). The question is what state(s) fit(s) the data in optimal way. One might be tempted to sample and invert the probability, predicted by quantum theory, as it is done in the case of equation (5). Because each SG detection is represented by a complete measurement, the sum the relations (6) for each setting of SG apparatus \(j\) reads

\[
\frac{1}{M} \sum_{j}^{M} |a^j\rangle\langle a^j| + |\!\!-a^j\!\!\rangle\langle -a^j| = \hat{1}.
\]

However, the expected relations

\[
\text{Tr}\{\hat{\rho} \frac{1}{M} |\pm a^j\rangle\langle \pm a^j|\} = \frac{1}{2M} (1 \pm X_j).
\]

cannot be fulfilled, in general, since the system is overcompleted and data are fluctuating. Hence, the probabilities cannot be mapped so straightforwardly with the relative frequencies of outcomes.

MaxLik principle provides a tool, how to treat this problem. The most probable state consistent with the data should be found. As the measure of probability, the likelihood functional corresponding to the product of all the probabilities for all detected data may be constructed

\[
\mathcal{L}(\hat{\rho}) = \prod_{j} \left(\frac{\langle a^j|\hat{\rho}|a^j\rangle}{(\langle a^j|\hat{\rho}|a^j\rangle + \langle a^j|\hat{\rho}|a^j\rangle)}\right)^{N(1+X_j)/2} \left(\frac{\langle -a^j|\hat{\rho}|-a^j\rangle}{\langle -a^j|\hat{\rho}|-a^j\rangle}\right)^{N(1-X_j)/2}.
\]

Extremal states of likelihood functional satisfy the nonlinear operator equation (11):

\[
\frac{1}{2M} \sum_{j} \left[ (1 + X_j) \frac{|a^j\rangle\langle a^j|}{(\langle a^j|\hat{\rho}|a^j\rangle + \langle a^j|\hat{\rho}|a^j\rangle)} + (1 - X_j) \frac{|-a^j\rangle\langle -a^j|}{\langle -a^j|\hat{\rho}|-a^j\rangle} \right] \hat{\rho} = \hat{\rho}.
\]

Quantum state may be represented by polarization. Using the relation (15), multiplying both the sides by \(a_k\) and performing the trace, the equation reads

\[
R(r)r + K(r) + iK(r) \times r = r,
\]

where the functions are defined as

\[
R(r) = \frac{1}{2M} \sum_{j} \left( \frac{1 + X_j}{1 + a^j r} + \frac{1 - X_j}{1 - a^j r} \right),
\]

\[
K(r) = \frac{1}{2M} \sum_{j} \left( \frac{1 + X_j}{1 + a^j r} - \frac{1 - X_j}{1 - a^j r} \right) a^j.
\]

Because real and imaginary parts are dependent, the real part of this equation represents sufficient and necessary conditions. The final equation for polarization reads

\[
R(r)r + K(r) = r.
\]
MaxLik fitting of an unknown quantum state inside the Poincaré sphere.

An equivalent result may be derived, provided that likelihood function is parameterized directly using the polarization. The relevant part of the likelihood function corresponding to the observation of particular data reads

\[ \mathcal{L}(\mathbf{r}) = \prod_j (1 + r a_j) \frac{N}{2} (1 - r a_j)^{-N/2}. \]  

The vector \( \mathbf{r} \) parameterizes an unknown polarization inside the Poincaré sphere and the products runs over all \( M \) directions. The standard statistical approach using MaxLik \( \frac{\partial}{\partial \mathbf{r}} \ln \mathcal{L} \) provides the vector equation for extremal polarization

\[ \sum_j X_j - a_j r = 0. \]  

The equation (14) is equivalent to the equation (13). Indeed, the equation (14) is nothing else as \( K(\mathbf{r}) = 0 \), implying the relation \( R(\mathbf{r}) = 1 \). On the other hand, the equation (14) may be rewritten to the form of equation (13) as well.

Results of numerical simulation are shown in the Fig. 1. Stern-Gerlach detection is simulated here for projection of an unknown state (north pole on Poincaré sphere) in five various directions. Each measurement is done with 20 impinging particles, which are registered either with the spin up (upper left panel) or down (lower left panel). Both the left panels show typical values for a single experiment. For each position of the projector there are three bars in the upper and lower left panels. The first bars (black) show the true value of the probability. The second bars (gray) show the counted statistics fluctuating around the true value of probability. The third bars (hollow) show results of the reconstruction – the statistics of reconstructed state corresponding to the given projector. Notice here, that upper and lower panels are complementary and sum of corresponding probabilities is one. The right panels visualize results of 10 times repeated experiment on the Poincaré sphere. Symbols of diamonds denote the positions of five projectors. Orthogonal projectors in opposite directions are not depicted. The stars show the position of reconstructed states. The true state corresponds to the north pole. Lower right panel show the upper view.

Quantum formulation posse a nontrivial interpretation, which can hardly be recognized in the equation for polarization (14). Because the above scheme determines a quantum state, it must exist a generalized measurement described by a probability operator measure (POM) \( \hat{a} \), result of which the quantum state is. Really, such a probability operator measure can be easily find by proper renormalization of original SG measurement \( \hat{a} \). Let us define the POM as renormalized SG projectors

\[ |\pm a|^2, \langle \pm a| = \frac{1}{2M} \frac{X_j}{|\hat{\rho}_{a}^j| a_j \langle \pm a|}. \]  

for each index \( j \). The closure relation then reads

\[ \sum_j |a_j|^2, \langle \pm a| R + |a_j\rangle \langle \pm a| R = \hat{1}, \]  

and the renormalized POM fulfills the conditions

\[ \text{Tr} \{ \hat{\rho}_{a}^j |\pm a| \langle \pm a| R \} = \frac{1}{2M} (1 + X_j). \]  

Here \( \hat{\rho}_{a} \) denotes the extremal state – a solution of the equation (14). Indeed, the relation (18) coincides with the equation for extremal states (12), whereas the condition for expectation values (19) is fulfilled as an identity. The reconstruction is done on the subspace, where the renormalized POM reproduces the identity operator. Particularly, this means that the identity operator on the right hand side of (18) is spanned by the one dimensional subspace only (i.e by a single ray), provided that the extremal state \( \hat{\rho}_{a} \) is a pure state. For a general extremal density matrix, the reconstruction is accomplished in the whole two dimensional Hilbert space. The distinction between relations (14), (15) and (18), (19) characterize the subtle point of quantum state reconstruction. MaxLik solution may be also interpreted in the language of probabilities. The detected data \( n_{i,\pm} \) samples different binomial probability distributions for \( i = 1, \ldots, M \). MaxLik estimation finds a common multinomial distribution, sampling of which the data seems to be with the highest likelihood.

The method developed here may be compared with the existing approaches. Jaynes maximum entropy principle (MaxEnt) \( (10) \) has been applied to the estimation of spin 1/2 states in Refs. (8), (3). In general, these methods are not equivalent. The MaxLik solution seeks for the most likely solution consistent with the data, whereas the MaxEnt searches for the worst solution still consistent with the data. This may be interpreted as different prior information in the maximum probability principle \( (11) \). But this is not the only difference. External conditions of both the approaches differ substantially. MaxLik has been applied to the measurements with many projectors. However, the same conditions cannot be used in MaxEnt principle. Since there are only three free parameters necessary for determination of an unknown spin state, conditions (10) cannot be fulfilled, in general. MaxEnt principle cannot be used provided that there are more than three independent conditions put on the density matrix of 1/2 spin system.

In the papers Refs. (3) an optimal strategy for measuring an unknown two-state system prepared in a mixed state is investigated. As a result, an optimal POM may be predicted. On the other hand, not the measurement but the mathematical treatment is optimized in this paper. This seems to be reasonable from the experimentalist’s point of view since it is questionable how to do a general measurement described by a POM. As demonstrated, for given measurement MaxLik estimation pro-
vides an optimal treatment, since it reproduces a quantum measurement. As argued in Ref. [13] both the treatments provide comparable results.

III. SUMMARY

Synthesis of incompatible observations represented by various settings of SG apparatus has been evaluated using MaxLik estimation. As the result it defines a generalized measurement of a quantum state. Synthesis of various incompatible observations is again a generalized measurement. Developed formalism will be applied in the future for investigation of various problems such as: spin estimation of neutrons in the depolarization experiments, estimation of quantum state inside the interferometer or analysis of entanglement.

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