Measurement theory for spinor condensates

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Abstract. We study the experimental signatures of several states of a Bose-Einstein condensate of spin-1 atoms by quantum trajectory simulations of Stern-Gerlach experiments. The measurement process itself creates an apparent random alignment for the spins, so that it is difficult to distinguish between a condensate that initially has an alignment in an unknown direction and one with no alignment at all. Nonetheless, in repeated experiments with identically prepared condensates, it is possible to discriminate between certain ground states of the condensate proposed in the literature.

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1. Introduction

With the introduction of the optical trap in the experiments on Bose-Einstein condensation, simultaneous confinement of atoms in several angular momentum states is now feasible [1]. The atomic spins interact in spin-exchange collisions, which gives rise to collective many-spin states. Energy differences between several conceivable ground states of the spinor condensate [2, 3, 4] have turned out to be small, so that it need not be obvious which one gets prepared in an experiment.

On the other hand, resolving the contradicting opinions of the past [5, 6], recent analyses have shown [7, 8, 9] that a Bose-Einstein condensate may display signatures of spontaneously broken gauge symmetry, such as interference of two independently prepared condensates [10] or the Josephson effect, even if the gauge symmetry of the state is in fact not broken. The lesson is that the relation between the state of the system and the measurement results may be conditioned as much by the experiment as by the state itself. How to distinguish experimentally between the proposed states of the spinor condensate [3, 4] is therefore a nontrivial question in its own right.

In this paper we study the experimental signatures of a spin-1 condensate for three different initial states, “coherent state” with spontaneous alignment [4], “fragmented state” in which there are two macroscopically occupied spin states [4], and rotationally invariant “singlet state” [3]. Our main tool is quantum trajectory simulations [11, 8, 9] of repeated Stern-Gerlach experiments. Once more [7, 8, 9], the interplay between state and measurement is evident. It appears that the coherent and fragmented states are experimentally indistinguishable, but can be distinguished easily from the singlet state. We also present a testable prediction for the distribution of the outcomes of the Stern-Gerlach experiments that probes the statistic of spin projections to all orders, not just averages and standard deviations. Finally, as an important by-product of our development we note that, while the simulations at first sight only apply to a quite artificial experimental scheme, they implement what we believe is a universal theory for spin measurements on a condensate.

2. States of spinor condensate

We consider putative ground states for the spinor condensate in the case when the spin species do not separate, but the atoms with the three angular momentum projections $m = \pm 1$ and $m = 0$ commingle with identical spatial wave functions. We assume scattering lengths such that the interaction between the spins is effectively antiferromagnetic. For brevity we assume zero magnetic field. Nonetheless, we still pick a quantization axis $z$. We write the annihilation operators for the atoms with the three spin components along the quantization axis as $a_\pm$ and $a_0$. For notational simplicity, we take the total number of atoms $N$ to be even.

The coherent state is arrived at via the semiclassical argument, which treats the annihilation operators $a_\pm$ and $a_0$ as $c$ numbers [4]. The $c$ numbers come with phases
that are not uniquely determined by minimization of energy. Assigning a value for the phases is tantamount to inserting by hand a form of spontaneous symmetry breaking. The corresponding quantized ansatz for the state of the spinor condensate reads [4]

$$|C\rangle = \frac{1}{\sqrt{2^N N!}} \left( e^{-i\chi a^\dagger_-} + e^{i\chi a^\dagger_+} \right)^N |\text{vac}\rangle. \quad (1)$$

Positing the state $|C\rangle$ is analogous to assuming that a single-component condensate is in a coherent state, as opposed to, say, a number state of the atoms [4, 5, 6]. $\chi$ is an angle that characterizes the symmetry breaking. It selects preferred directions in the $xy$ plane.

The fragmented or “coherent-fragmented state” [4] is just a number state with half of the spins in the state $+\,$ and half in the state $-\,$,

$$|F\rangle = |N/2, 0, N/2\rangle. \quad (2)$$

The arguments give the numbers of atoms with the $z$ components of the angular momentum equal to $-1, 0, \text{ and } +1$. In the thermodynamic limit the state $|F\rangle$ should model the ground state in the presence of even the most minute magnetic field in the $z$ direction [4]. While this state could behave differently in the $x$ and $z$ directions, it has no built-in structure in the $xy$ plane.

The singlet state of [3] is of the form

$$|S\rangle = \sum_{k=0}^{N/2} A_k |k, N - 2k, k\rangle. \quad (3)$$

The coefficients $A_k$ satisfy the recursion relation

$$A_k = -\sqrt{\frac{N - 2k + 2}{N - 2k + 1}} A_{k-1}, \quad (4)$$

and are then fixed by normalization, except for an arbitrary overall phase. The state $|S\rangle$ is the unique ground state for exactly zero magnetic field. It has the same form in all rotated frames, and thus possesses no intrinsic direction.

### 3. Measurements on spins

In our model for the measurements, we assume for the time being that one atom at a time is removed from the condensate and is subject to a Stern-Gerlach experiment that probes the spin component in the $xy$ plane in a fixed direction at an angle $\phi$ with respect to the $x$ axis. The observed sequence of spin projections is recorded and analyzed. All measurements are supposed to be completed in a time shorter than the evolution time scale of the spins in the condensate owing to spin-spin interactions.

From angular momentum algebra it is easy to see that the annihilation operators for the spin states in the direction $\varphi$ are given in terms of the original quantization axis operators as

$$a_{\pm}(\varphi) = \frac{e^{i\varphi}}{2} a_- \pm \frac{1}{\sqrt{2}} a_0 + \frac{e^{-i\varphi}}{2} a_+ , \quad (5)$$
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\[ a_0(\varphi) = \frac{e^{i\varphi}}{\sqrt{2}} a_- - \frac{e^{-i\varphi}}{\sqrt{2}} a_+ . \]  

(6)

We carry out conventional quantum trajectory simulations of the measurement sequence \[8, 9\] numerically. Thus, suppose that, entering the \(n\)th measurement, the normalized state of the spins is \(|\psi_n\rangle\). We first calculate the probabilities for each spin projection,

\[ P_m^{(n)} = \frac{\langle \psi_n | a_m^\dagger(\varphi) a_m(\varphi) | \psi_n \rangle}{N - n} \]  

(7)

for \(m = -1, 0\) and \(+1\). Second, we use a random number generator to pick one of the \(m\) values in such a way that the probability for choosing \(m\) equals \(P_m^{(n)}\). Third, we reduce the wave packet according to the selected value of \(m\), so that the state vector for the \((n + 1)\)th measurement is

\[ |\psi_{n+1}\rangle = \frac{a_m(\varphi) |\psi_n\rangle}{\sqrt{\langle \psi_n | a_m^\dagger(\varphi) a_m(\varphi) | \psi_n \rangle}} . \]  

(8)

The choices of the spin projection \(m\) for each measurement \(n\) constitute the data.

We first consider the coherent state, \(|\psi_0\rangle = |C\rangle\). It turns out that, except for an inconsequential overall phase, and independently of the past choices of the spin projections, the state vector \(|\psi_n\rangle\) is always a coherent state of the same form as \(|C\rangle\), except that of course the total number of atoms is \(N - n\) not \(N\). Furthermore, the probabilities for the outcomes of the Stern-Gerlach experiment are always the same,

\[ P_\pm^{(n)} = \frac{1}{2} \cos^2(\varphi - \chi), \quad P_0^{(n)} = \sin^2(\varphi - \chi). \]  

(9)

Successive Stern-Gerlach experiments are therefore uncorrelated. The nature of the symmetry breaking is alignment. Namely, in the measurement directions \(\varphi = \chi \pm \frac{1}{2}\pi\) one only sees the result \(m = 0\), whereas in the directions \(\varphi = \chi\) and \(\varphi = \chi + \pi\) one finds \(m = \pm 1\) with equal probabilities, and no \(m = 0\).

Now, according to the notion of spontaneous symmetry breaking, the angle \(\chi\) varies at random from one spinor condensate to the next, and the experimenter has no a priori way of knowing it. As the observed frequencies of spin projections \(N_0, N_\pm\) vary wildly with the angle \(\chi\), measurements on just a single condensate do not seem to make a particularly discriminating test for or against the state \(|C\rangle\).

To gather more incisive data, we imagine repeating the experiment with a large number of identically prepared condensates. In principle we should discuss the frequencies of the observed spin projections, but in our simulations we have access to the probabilities \(P_0^{(n)}\) and \(P_\pm^{(n)}\) as well. For brevity, here we often pick a particular measurement \(n\), and focus on the combination of the probabilities

\[ P = P_-^{(n)} + P_+^{(n)} - P_0^{(n)}. \]  

(10)

For a given condensate in the coherent state \(|C\rangle\) this has the value \(P = \cos^2(\varphi - \chi) - \sin^2(\varphi - \chi)\), but the angle \(\chi\) is unknown. Nonetheless, if the angle \(\chi\) is evenly distributed
over the unit circle $[0, 2\pi)$, we may calculate the probability density $f(P)$ for the values of $P$. The result is

$$f(P) = \begin{cases} \frac{1}{\pi \sqrt{1 - P^2}}, & P \in (-1, 1); \\ 0, & \text{otherwise.} \end{cases} \tag{11}$$

Thus, we envisage using a large number of condensates. For each condensate one extracts the combination of probabilities $P$, in our numerical experiments using (10) for some given measurement $n$, and in real experiments by estimating the probabilities using the observed frequencies of spin projections for each condensate. Finally one compares the distribution of the numbers $P$ with predictions such as (11). In the case of the coherent state $|C\rangle$, the numerical experiments simply amount to testing of our algorithms.

We next move on to the fragmented state $|F\rangle$. In figure 1(a) we plot the numerically simulated probabilities $P^{(n)}_0$ and $P^{(n)}_\pm$ as a function of the measurement number $n$ for a sample condensate with $N = 1000$ atoms, and figure 1(b) gives the corresponding cumulative frequencies $N_0$, $N_\pm$. Notably, after an initial transient, the probabilities approximately stabilize at values compatible with the observed relative frequencies of the spin components.

The expectation values for the numbers of spins with given projections are

$$\langle a_\dagger_\pm(\phi)a_{\pm}(\phi) \rangle = \frac{1}{2}N, \quad \langle a_0(\phi)a_0(\phi) \rangle = \frac{1}{4}N.$$  

One might naively expect that, even in a single condensate, one would find the spins approximately in the ratio $N_- : N_0 : N_+ = 1 : 2 : 1$. This clearly is not the case. In figure 1(b) the ratios rather are $2:1:2$. Moreover, the observed ratios vary at random from one condensate to another.

The measurements are correlated; the outcome of an observation of the projection of a spin affects the state, which in turns affects the outcome of future observations. The correlations work out in an interesting way. In the first measurement the probabilities are $\frac{1}{4} : \frac{1}{2} : \frac{1}{4}$, but then they quickly drift away and stabilize at some other values. Once the probabilities have stabilized, Stern-Gerlach measurements seem to be approximately independent repetitions of one another. However, the apparent state that is being repeatedly measured varies at random from one condensate to the other. Measurements on the fragmented state $|F\rangle$ in an individual condensate behave remarkably like measurements on the symmetry-broken coherent state $|C\rangle$.

It is legitimate to ask if the states $|F\rangle$ and $|C\rangle$ can be distinguished at all. We address this question further in figure 2. We take 1000 spinor condensates, each with $N = 500$ atoms. For each condensate we record the quantity $P$ of (10) for the Stern-Gerlach measurement number $n = 101$. We then bin the results into 40 equally wide slots of $P$, and draw the histogram as circles. Also shown as the solid line is the prediction for the histogram if the probability distribution for the values of $P$ is given by (11), as appropriate for the coherent state $|C\rangle$. Given the statistical fluctuations, we cannot tell the states $|F\rangle$ and $|C\rangle$ from one another.

The situation is remarkably similar to the one that was encountered earlier with a single-component condensate when it came to the question of a number state, versus a
Figure 1. Simulated probabilities (a) and cumulative frequencies (b) for spin projections as a function of measurement number in one particular condensate that starts out with 1000 atoms in the fragmented state $|F\rangle$.  
coherent state whose phase arises from spontaneously broken gauge symmetry \[7, 8, 9\]. When detection of the atoms is explicitly considered, it turns out that both states lead to interference between independently prepared condensates, even though the number state seemingly does not provide any phase for the interference \[7, 8\]. Both coherent-state and number-state condensates even exhibit the Josephson effect \[9, 12\]. It is possible in principle to tell the difference between a coherent state and a number state by studying atom statistics for a small number (at most tens) of atoms \[13\], but an experiment discriminating between coherent and number states is yet to be carried out in a condensate of any size. We believe that, analogously, there would be little or no practical difference between the states \(|C\rangle\) and \(|F\rangle\) of the spinor condensate.

Let us finally consider the singlet state \(|S\rangle\). The expectation values of the spin components are all \(\langle a_\pm^\dagger(\varphi)a_\pm(\varphi)\rangle = \langle a_0^\dagger(\varphi)a_0(\varphi)\rangle = \frac{1}{3}N\). However, just like in the case of the fragmented state \(|F\rangle\), in a single condensate both the simulated probabilities and the frequencies stabilize at values that may be completely different from \(N_- : N_0 : N_+ = 1 : 1 : 1\). One may, of course, draw a histogram such as in figure 2 also for the state \(|S\rangle\), which we have done in figure 3. The discrepancy with the prediction of the coherent state \(|C\rangle\) is evident even without any statistical analysis.

Drawing the histogram for the state \(|S\rangle\) might already have been a case of
overkill. While the frequencies for spin projections are seemingly random for a single condensate, we have found that they behave as expected when averaged over many condensates: 1 : 2 : 1 for the states $|C\rangle$ and $|F\rangle$, 1 : 1 : 1 for the state $|S\rangle$. The singlet $|S\rangle$ should be experimentally distinguishable from the other two states simply by averaging the frequencies of spin projections over many condensates.

4. Comparing schemes for Stern-Gerlach experiments

Up to now we have envisaged picking one atom at a time out of the condensate. In reality one might rather do an en masse Stern-Gerlach experiment, subjecting the entire spinor condensate at once to a gradient of the magnetic field. The spin projections then separate in space, and can be counted by counting atoms.

We assume that the detection is in principle still one atom at a time, as if the atoms fell on small detectors like photons hitting silver bromide grains on a photographic film. It is known from the theory of photon detectors \cite{14} that the joint counting rate of an array of absorbing broadband detectors is proportional to normally ordered correlation functions of electric field operators. Analogously, we conjecture that the joint probability of seeing a sequence of spin projections $m_1, m_2, \ldots, m_N$ is given by

$$P(m_1, \ldots, m_N) = K \langle a_{m_1}^\dagger(\varphi) \cdots a_{m_N}^\dagger(\varphi) a_{m_N}(\varphi) \cdots a_{m_1}(\varphi) \rangle,$$

where $K$ is the normalization constant needed to make the sum of all probabilities...
equal to unity. In photon detection theory the electric field operators are in time order as well, but inasmuch as we assume that we may ignore the reversible evolution of the spins during the measurement, the annihilation (creation) operators in (12) are taken at the same time and commute. The joint probabilities are then independent of the order of the indices $m_1, \ldots , m_N$, i.e., independent of the order in which the atoms are detected.

Suppose that the spin system starts out with the state vector $|\psi_0\rangle$, and consider the correlation functions as in (12). We may, of course, write

$$
\langle \psi_0 | a^\dagger_{m_1} (\varphi) \cdots a^\dagger_{m_N} (\varphi) a_{m_N} (\varphi) \cdots a_{m_1} (\varphi) | \psi_0 \rangle
$$

$$
= \left[ \langle \psi_0 | a^\dagger_{m_1} (\varphi) \right] a^\dagger_{m_2} (\varphi) \cdots a^\dagger_{m_N} (\varphi) a_{m_N} (\varphi) \cdots a_{m_2} (\varphi) \left[ a_{m_1} (\varphi) | \psi_0 \rangle \right].
$$

(13)

Trivial as this rewrite is, it immediately leads to two crucial observations. First, in (12) the probabilities for the various outcomes $m_1$ are precisely as given by (7) for $n = 1$. Second, once any particular value $m_1$ has been picked, the process starts over; we are left with the correlation functions

$$
\langle \psi_1 | a^\dagger_{m_2} (\varphi) \cdots a^\dagger_{m_N} (\varphi) a_{m_N} (\varphi) \cdots a_{m_2} (\varphi) | \psi_1 \rangle
$$

where the new state $|\psi_1\rangle$ is the $n = 1$ version of (8). We have thus shown that our quantum trajectory simulations produce spin sequences $m_1, \ldots , m_N$ that have the probabilities predicted by (12). A fortiori, the results from quantum trajectory simulations agree with the predictions of (12).

Our simulations were seemingly for a scheme in which one atom at a time is subject to a Stern-Gerlach experiment. We did not offer any concrete suggestions on how to carry out such experiments, but neither did we have to. Inasmuch as our reasoning leading to (12) is correct, our simulations also model the usual [1] Stern-Gerlach measurements on the spinor condensate.

One might also study the number operators for different spin projections, such as $n_0 (\varphi) = a^\dagger_0 (\varphi) a_0 (\varphi)$, in total disregard of the measurement process. As far as we can tell, our quantum trajectory simulations averaged over many condensates give the same qualitative and semi-quantitative results that one would expect on the basis of elementary quantum mechanics with the operators $n_0 (\varphi), n_{\pm} (\varphi)$.

As a qualitative example, the fluctuations of $n_0 (\varphi)$ in the state $|F\rangle$ are large, $\Delta n_0 \simeq \sqrt{\frac{1}{N} n}$. In quantum trajectory simulations one correspondingly sees wildly varying ratios in the frequencies of spin projections between individual condensates. From this viewpoint, measurement-induced alignment is the reason for the large fluctuations in $n_0 (\varphi)$ [and $n_{\pm} (\varphi)$]. More quantitatively, one may compute the expectation value and the standard deviation for the number of atoms with a given spin projection in a condensate either by using quantum mechanics with the operators $n_0 (\varphi)$, etc., or by averaging over quantum trajectory simulations of a large number of condensates. We have found that, for large $N$, the results agree.
5. Concluding remarks

Both quantum trajectory simulations and (12) give seemingly sensible predictions for the frequencies of spin projections and their fluctuations even for the en masse Stern-Gerlach experiment. But they do a lot more, too. For instance, a histogram such as in figure 2 may be prepared for the results of en masse experiments and compared with the predictions of quantum trajectory simulations. Such a histogram probes the spin statistics in principle to all orders, beyond average and standard deviation. We thus have a nontrivial prediction from (12) that may be contrasted with experiments.

Another possible extension of our method is time evolution, as in the Josephson effect [9] or in the time dependence of spin correlations. We may straightforwardly incorporate time ordering and time evolution of the annihilation operators into (12). In contrast, an approach in terms of the number operators $n_0(t), n_{\pm}(t)$ without an explicit consideration of the measurements probably makes a subtle affair [12].

It would seem worthwhile to derive (12) from microscopic arguments [15], along the lines of earlier work on photons [14]. To the extent that this can be done, our quantum trajectory simulations would be proven to be a universal method for the studies of the detected properties of a spinor condensate. More generally, coherence theory of light is built entirely on the theory of photon detection, so it appears plausible that the eventual coherence theory for Bose-Einstein condensates is based on detection theory as well. The combination of measurement theory and accompanying quantum trajectory simulations is at present our best bet for a general approach to the coherence properties of a condensate.

In sum, we have laid down a measurement theory and the accompanying quantum trajectory simulations for a spinor condensate, and proposed a nontrivial experiment in which our approach may be tested. The main result thus far is that the state of the spinor condensate and measurements thereof are intertwined to the extent that it is probably impossible to distinguish experimentally between the symmetry-broken coherent state and the fragmented state of the condensate. In the process we have uncovered new aspects of measurement theory which should prove fruitful in future discussions of the coherence properties of a condensate.

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