RELATIVE PHASE STATES IN QUANTUM–ATOM OPTICS
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0.1 Abstract

Relative phase is treated as a physical quantity for two mode systems in quantum atom optics, adapting the Pegg-Barnett treatment of quantum optical phase to define a linear Hermitian relative phase operator via first introducing a complete orthonormal set of relative phase eigenstates. These states are contrasted with other so-called phase states. Other approaches to treating phase and previous attempts to find a Hermitian phase operator are discussed. The relative phase eigenstate has maximal two mode entanglement, it is a fragmented state with its Bloch vector lying inside the Bloch sphere and is highly spin squeezed. The relative phase states are applied to describing interferometry experiments with Bose-Einstein condensates (BEC), particularly in the context of a proposed Heisenberg limited interferometry experiment. For a relative phase eigenstate the fractional fluctuation in one spin operator component perpendicular to the Bloch vector is essentially only of order $1/N$, so if such a highly spin squeezed state could be prepared it may be useful for Heisenberg limited interferometry. An approach for preparing a BEC in a state close to a relative phase state is suggested, based on adiabatically changing parameters in the Josephson Hamiltonian starting from a suitable energy eigenstate in the Rabi regime.
1 Introduction

Studies of phase dependent phenomena in Bose-Einstein condensates (BEC) are hindered because phase has at least three different meanings. A similar situation applies in quantum optics [1]. In a first approach, phase is regarded as a physical property of the system [2] and is represented via a linear Hermitian operator that applies for all states and for which phase is the (real) eigenvalue. In a second treatment, the state is represented in a phase space [3], [4] by a quasi-distribution function, and a complex phase is used to specify points in this space. In a third method, an operational approach [5], [6] emphasises an apparatus involved in measurements on the system and phase then refers to a feature of this measurement apparatus, such as the phase of a classical oscillator field interacting with the system. The dependence of system behaviour on phase in these three approaches are different in general, making comparison difficult because the meaning of "phase" is not the same. In a simple example presented in [1], it is shown that no quantum state leads to a uniform phase dependence for all three different meanings for phase. It is important therefore to recognise that phase is different in the three approaches. Choosing which approach to use is somewhat a matter of personal preference, but from a fundamental point of view treating phase in the same way as other physical quantities would be preferable - if possible. The operational phase approach has the disadvantage of not linking phase to any intrinsic property of the system, and is dependent on the choice of apparatus. This generally involves some sort of homodyne system, but various combinations of beam splitters, phase shifters, vacuum input ports, detectors etc can also be involved. The phase space approach involves a complex phase which cannot be a measured value for any physical quantity and is dependent on the choice of distribution function used to describe the state. This could be Wigner W, Glauber-Sudarshan P, Husimi Q, or other distributions. In fact the complex phase is often the eigenvalue of a non-Hermitian annihilation operator, which cannot represent a physical quantity. In neither of these two approaches is there any unique or compelling choice for defining phase. Thus the introduction of phase via eigenvalues of a linear Hermitian operator associated with the quantum system is the most objective approach [1] because it is not dependent on any particular way of specifying the state nor on any particular measurement system. This is not to claim that some ways of specifying the state are not more useful than others, nor is it intended to trivialise the difficult issue of measuring the probability distribution for the measurable values of phase regarded as a physical property. Nor does it prove easy to find a suitable Hermitian operator to represent phase. However such an operator can now be defined both for quantum optical systems and Bose-Einstein condensates following the approach of Pegg and Barnett [2] that was originally applied to the quantum optics case (see [7] for a recent review).

In the present paper we begin with a brief review of progress towards finding
a Hermitian phase operator, and then the Pegg-Barnett approach is adapted to define a relative phase operator for two mode systems via first introducing a complete orthonormal set of relative phase eigenstates. These states are contrasted with other so-called phase states. Interesting properties of the relative phase eigenstates are then determined, these being entanglement, fragmentation and spin squeezing. In the final section applications of the relative phase states in describing BEC interferometry experiments are made based on treatment involving the Josephson Hamiltonian, and possibilities for preparing a BEC in a relative phase state are examined. Certain technical results needed for the main body of the paper are covered in an Appendix, which is available as online Supplementary Data.

2 Hermitian phase operators

2.1 Early attempts

Early attempts to find a Hermitian phase operator for each mode by expressing the annihilation and creation operators $\hat{a}$, $\hat{a}^\dagger$ in terms of Hermitian number operator $\hat{n}$ and phase operator $\hat{\phi}$ via $\hat{a} = \exp(i\hat{\phi}) (\hat{n})^{1/2}$, $\hat{a}^\dagger = (\hat{n})^{1/2} \exp(-i\hat{\phi})$ with $[\hat{\phi}, \hat{n}] = -i$ were unsuccessful. For the first, the commutation rule leads to a contradiction when matrix elements between number states are evaluated $\langle n - m | \hat{n} | n \rangle = -i\delta_{nm}$. For the second, the introduction of a Hermitian phase operator required being able to write $\hat{E}^+ = (\hat{n} + 1)^{-1/2} \hat{a}$, $\hat{E}^- = \hat{a}^\dagger (\hat{n} + 1)^{-1/2}$ were unsuccessful. For the first, the commutation rule leads to a contradiction when matrix elements between number states are evaluated $\langle n - m | \hat{n} | n \rangle = -i\delta_{nm}$. For the second, the introduction of a Hermitian phase operator required being able to write $\hat{E}^+ = \exp(i\hat{\phi})$ and $\hat{E}^- = \exp(-i\hat{\phi})$ in the form of unitary operators also failed, for although $\hat{E}^+\hat{E}^- = \hat{1}$ we have $\hat{E}^-\hat{E}^+ = \hat{1} - |0\rangle \langle 0|$ - rather than $\hat{1}$ as is required. Note that Hermitian cosine and sine operators $\hat{C}$, $\hat{S}$ can be introduced via $\hat{E}^+ = \hat{C} + i\hat{S}$, but again these are not trigonometric functions of a Hermitian phase operator. However, the approach of Pegg and Barnett via the introduction of phase eigenstates and then the Hermitian phase operator was successful. This approach does require introducing a cut-off on boson numbers for each mode, but this can be justified mathematically in terms of a sequence of Hilbert spaces and shown not to affect physical predictions for finite energy fields.

2.2 Relative phase operator and eigenstates

In this section we introduce relative phase eigenstates and a Hermitian relative phase operator for the case of a two mode single component BEC with mode annihilation operators $\hat{a}$, $\hat{b}$ and spatial mode functions $\phi_a(r)$, $\phi_b(r)$ using a modification of the Pegg-Barnett approach for single modes. From the Fock state orthonormal basis states $|n_a\rangle$, $|n_b\rangle$ involving $n_a$, $n_b$ bosons in the modes a complete orthonormal set of relative phase eigenstates $|\theta_P\rangle$ for the $N = n_a + n_b$...
boson system are then defined via
\[ |\theta_p\rangle = \frac{1}{\sqrt{N+1}} \sum_{k=-N/2}^{N/2} \exp(ik\theta_p) |N/2-k\rangle_a |N/2+k\rangle_b \] (1)
where \( \theta_p = p(2\pi/(N+1)) \), \( p = -N/2, -N/2 + 1, \ldots, +N/2 \) is a quasi-continuum of \( N + 1 \) equispaced phase eigenvalues. The Hermitian relative phase operator is then defined as
\[ \hat{\Theta} = \sum_p \theta_p |\theta_p\rangle \langle \theta_p| \] (2)
This approach has also been applied previously in [12], [13]. Also an un-normalised version of Eq.(1) with phase angle \( -\theta_p \) is introduced in [14] (see Eqs. A3 and A4). The relative phase operator defined in (2) depends on the choice of modes and the total boson number \( N \), and its commutation law with the relative number operator \( \hat{n} = \frac{1}{2}(\hat{b}^\dagger \hat{a} - \hat{a}^\dagger \hat{b}) \) is
\[ [\hat{\Theta}, \hat{n}] = i \sum_{p \neq q} \theta_p \theta_q (-1)^{p-q} \frac{(\theta_p - \theta_q)^2}{\sin(\theta_p - \theta_q)^2} \]
rather than just \( i \). The Fock state \( |N/2-k\rangle_a |N/2+k\rangle_b \) is an eigenstate of the relative number operator with eigenvalue \( k \). Note that the present approach for a two mode system defines a relative phase eigenstate and relative phase operator, rather than phase eigenstates and operator for each mode. However, the relative phase operator can be defined without requiring a cut-off on boson numbers since there is an automatic restriction for \( k \) to lie between \( -N/2 \) and \( +N/2 \). The definition can be extended to apply to mixed state boson systems with a range of \( N \) via \( \hat{\Theta}_T = \sum_N \hat{\Pi}_N \hat{\Theta}(N) \hat{\Pi}_N \) using projectors \( \hat{\Pi}_N \) onto \( N \) boson states. Note that essentially the same states can also be defined for quantum optical systems, there the bosons are massless photons.

An approach closer to the original Pegg and Barnett method would be to define phase operators for each mode, and then the relative phase operator would be the difference between the separate phase operators for the two modes, and this method is used in Ref.[15]. This approach requires introducing a cut-off on boson numbers for each mode and special techniques are needed to restrict the phase difference to a \( 2\pi \) rather than \( 4\pi \) interval. There are differences between this approach and that adopted here and in [12], [13], which are discussed in [16], [17]. The approach presented here provides a more direct focus on relative phase as a basic physical property and enables the relative phase to automatically lie in a \( 2\pi \) interval.

A similar approach to that here can also be used to define relative phase eigenstates and a Hermitian relative phase operator for a two component BEC where each (hyperfine) component is associated with a single spatial mode function. This situation is again a two mode system and similar Fock states to \( |N/2-k\rangle_a |N/2+k\rangle_b \) act as an orthonormal basis, though now \( |n_a\rangle \) has \( n_a \) bosons in a spatial mode \( \phi_a(r) \) associated with internal (hyperfine) state \( a \).
2.3 Pure states and quantum superpositions

Any pure quantum state $|\Phi\rangle$ for the $N$ boson system can be expanded in terms of the relative phase states as

$$|\Phi\rangle = \frac{N/2}{\sqrt{N+1}} \sum_{p=-N/2}^{N/2} A(\theta_p) |\theta_p\rangle$$

and the amplitudes $A(\theta_p)$ determine the probability $P(\theta_p)$ for measuring the relative phase $\theta_p$ via the standard expression

$$P(\theta_p) = |A(\theta_p)|^2$$

The same state can also be expanded in terms of the relative number states as

$$|\Phi\rangle = \frac{N/2}{\sqrt{N+1}} \sum_{k=-N/2}^{N/2} b_k |N/2-k\rangle_a |N/2+k\rangle_b$$

with expansion coefficients $b_k$. It is then easy to see that the expansion coefficients in terms of relative phase states and the Fock states are related via a Fourier transform.

$$A(\theta_p) = \frac{1}{\sqrt{N+1}} \sum_k \exp(-ik\theta_p) b_k \quad b_k = \frac{1}{\sqrt{N+1}} \sum_p \exp(+ik\theta_p) A(\theta_p)$$

For the relative phase state itself the expansion coefficients are $b_k = \exp(+ik\theta_p)/\sqrt{N+1}$. The generalisation for mixed states is straightforward.

As an example of a quantum superposition we consider the state

$$|\Phi\rangle = \frac{1}{\sqrt{2}} \left( |N, 0\rangle_a |N, 0\rangle_b + |0, N\rangle_a |0, N\rangle_b \right)$$

which is the so-called NOON state, being a superposition of states $|N, 0\rangle$ and $|0, N\rangle$. It is also referred to as a Schrödinger cat state, and is an example of an entangled state. In the first term there are $N$ bosons in mode $\phi_L$ and 0 in mode $\phi_R$ and for the second the reverse applies. For this state $b_k = (\delta_{k,-N/2} + \delta_{k,+N/2})/\sqrt{2}$ and hence $A(\theta_p) = \sqrt{2/(N+1)} \cos(\frac{N}{2} \theta_p)$, which gives an oscillatory probability distribution for the relative phase with probabilities changing from 0 to $2/(N+1)$ for neighboring phase angles. Such oscillations would be hard to detect. On the other hand the different NOON state

$$|\Phi\rangle = \frac{1}{\sqrt{2}} \left( |N, 0\rangle_a |N, 0\rangle_b + |0, N\rangle_a |0, N\rangle_b \right)$$

with $n \ll N$ and $A(\theta_p) = \sqrt{2/(N+1)} \cos(n \theta_p)$ would have a central peak in the phase probability for $\theta_p = 0$ and the first zero at $\theta_p = \pm \pi/2n$, which would correspond to a relative narrow phase probability distribution with $\Delta \theta_p \propto 1/n$, if $n$ is large enough.
2.4 Other phase dependent states

Note that other authors [18] have defined a set of states for a two mode BEC that depend on phase variables $\theta$, $\chi$ via the expression

$$ |\theta, \chi\rangle = \frac{1}{\sqrt{N!}} \left( \cos \theta \cdot \exp(-\frac{i}{2} \chi) \hat{a}^\dagger + \sin \theta \cdot \exp(+i\frac{1}{2} \chi) \hat{b}^\dagger \right)^N |N\rangle_a |0\rangle_b $$

(9)

which are also referred to as phase states. For the case where $\theta = \pi/4$ such states have been used to define a phase $\chi$ in BEC interferometry experiments [19], and $\chi$ is measured in terms of the evolution time for a condensate in a double well trap when inter-well tunneling dominates over collisional effects. In this case phase is essentially the evolution time, which is an operational variable directly associated with the specific measurement process. However, states such as $|\theta, \chi\rangle$ are actually binomial states and correspond to all bosons being in the same single particle state $\cos \theta \cdot \exp(-\frac{i}{2} \chi) \phi_a(r) + \sin \theta \cdot \exp(+i\frac{1}{2} \chi) \phi_b(r)$. They are also referred to as coherent states. Expanding the coherent states

$$ |\theta, \chi\rangle = \sum_k b_k(\theta, \chi) |N/2 - k\rangle_a |N/2 + k\rangle_b $$

(10)

as a superposition of the basis states $|N/2 - k\rangle_a |N/2 + k\rangle_b$, the expansion coefficients are $b_k(\theta, \chi) = C^N_{N/2 - k} \cdot (\cos \theta)^{N/2 - k} \cdot (\sin \theta)^{N/2 + k} \cdot \exp(ik\chi)$ involving binomial coefficients $C^N_{N/2 - k} = N! / ((N/2 - k)!(N/2 + k)!).$ The binomial states are physically important since they describe an unfragmented BEC [20]. However they are not a complete orthonormal basis set for the two mode BEC. For example there is no choice of $\theta$, $\chi$ that gives the fragmented state $|N/2\rangle_a |N/2\rangle_b$ which has an occupancy for each of the two natural orbitals (see below) of $N/2$. For the coherent state with equal probabilities of finding a boson in each mode $|\theta = \pi/4, \chi\rangle$ the expansion [23] in terms of relative phase states $|\theta_p\rangle$ gives a relative phase probability

$$ P_{\pi/4, \chi}(\theta_p) = \sqrt{\frac{2\pi}{N}} \sqrt{\frac{N}{N + 1}} \exp \left( -\frac{N(\theta_p - \chi)^2}{2} \right) $$

(11)

for $N$ large. This is a Gaussian distribution centred around $\theta_p = \chi$ with a narrow width of $\Delta \theta_p \propto 1/\sqrt{N}$. For this coherent state the relative phase distribution corresponds to the standard quantum limit. Note that for large $N$ this coherent state almost has a well-defined relative phase $\chi$, which may explain why it is sometimes regarded as being a state with a definite relative phase. However, they are not eigenstates of any relative phase operator.

Other authors [21] consider eigenstates $|E(\theta)\rangle$ of a phase dependent quadrature operator for each mode $\hat{E}(\theta) = i(\hat{a} \exp(-i\theta) - \hat{a}^\dagger \exp(-i\theta))$ with eigenvalue $E(\theta)$, and probability distributions given as $| \langle E(\theta) | \Phi \rangle |^2$ for finding the quadrature field to have an amplitude $E(\theta)$ considered as a function of phase variable $\theta$ determine a phase distribution for a quantum state $|\Phi\rangle$ without introducing phase as an eigenvalue of a Hermitian operator. The expansion of the quadrature eigenstates in terms of Fock states $|n_a\rangle_a$ involves Hermite polynomials and
Gaussian functions of $E(\theta)$. However, the states $|E(\theta)\rangle$ are non-orthogonal so the probability concept is doubtful. This treatment of phase is really an example of the phase space approach.

3 Properties of relative phase eigenstates

The relative phase eigenstate has several interesting properties. These include entanglement, fragmentation and spin squeezing. We deal with each in turn.

3.1 Mode entanglement

Firstly, it is a state with maximal mode entanglement for the $a$, $b$ sub-systems, so is of interest in quantum information. The entropy of entanglement is one of the standard measures of entanglement [22] and is given by the von Neumann entropy for the reduced density operator for either of the subsystems $a$ or $b$. Thus for the system in pure state $|\Phi\rangle$ the entropy of entanglement is

$$S(\hat{\rho}_a) = -k_B Tr(\hat{\rho}_a \log \hat{\rho}_a) = -k_B Tr(\hat{\rho}_b \log \hat{\rho}_b) = S(\hat{\rho}_b)$$

$$\hat{\rho}_a = Tr_b(|\Phi\rangle \langle \Phi|) \quad \hat{\rho}_b = Tr_a(|\Phi\rangle \langle \Phi|)$$  \hspace{1cm} (12)

For the relative phase eigenstate it is straightforward to show that the entropy of entanglement is given by

$$S(\hat{\rho}_a) = k_B \log(N + 1) = S(\hat{\rho}_b)$$  \hspace{1cm} (13)

which is very large. The general case of maximal mode entanglement occurs when the amplitudes $b_k$ in (5) satisfy $|b_k| = 1/\sqrt{N + 1}$ [23], and the relative phase eigenstate is a particular case.

3.2 Fragmentation

Secondly, it is a fragmented state [20], since there are two natural orbitals with macroscopic occupancy. For large $N$ the first order quantum correlation function $G^{(1)}(r, r') = \langle \hat{\Psi}^\dagger(r)\hat{\Psi}(r') \rangle$ (where $\hat{\Psi}^\dagger(r), \hat{\Psi}(r)$ are the usual field operators, $\hat{\Psi}(r) = \hat{a}\phi_a(r) + \hat{b}\phi_b(r)$) is given by (see Appendix)

$$G^{(1)}(r, r') = \frac{N}{2} (\phi_a^*(r)\phi_a(r') + \phi_b^*(r)\phi_b(r'))$$

$$+ \frac{\pi N}{8} \exp(i\theta_p)(\phi_a^*(r)\phi_b(r')) + \frac{\pi N}{8} \exp(-i\theta_p)(\phi_b^*(r)\phi_a(r'))$$  \hspace{1cm} (14)

using the result that for large $N$ the sum $\sum_k \sqrt{(\frac{N}{2} - 1) - k(k \pm 1)/(N + 1)}$ is approximately $\frac{\pi N}{8}$. The natural orbitals are the eigenfunctions of the first order quantum correlation function, and are given by $\chi_{\pm}(r) = (\exp(i\theta_p/2)\phi_a^*(r) \pm$
3.3 Spin squeezing

Thirdly, the relative phase eigenstate is a spin squeezed state \[26\] in which one component of the spin angular momentum has a Heisenberg limited fluctuation. The Schwinger spin operators are defined by \[\hat{S}_x = (\hat{b}^\dagger \hat{a} + \hat{a}^\dagger \hat{b})/2, \hat{S}_y = (\hat{b}^\dagger \hat{a} - \hat{a}^\dagger \hat{b})/2i, \hat{S}_z = (\hat{b}^\dagger \hat{b} - \hat{a}^\dagger \hat{a})/2,\] and the Bloch vector is defined via its components \[\langle \hat{S}_x \rangle, \langle \hat{S}_y \rangle\] and \[\langle \hat{S}_z \rangle\] \[27\], often in units of \(N\). For large \(N\) the Bloch vector is determined to be (see Appendix)

\[
\langle \hat{S}_x \rangle \doteq \frac{\pi}{8} N \cos \theta_p \\
\langle \hat{S}_y \rangle \doteq -\frac{\pi}{8} N \sin \theta_p \\
\langle \hat{S}_z \rangle = 0
\]

using the result that for large \(N\) the sum \(\sum_k \sqrt{(\frac{N}{2} (\frac{N}{2} + 1) - k(k + 1)/(N + 1)})\) is approximately \(\frac{\pi}{8} N \doteq 0.3926N\). This vector is in the equatorial plane with azimuthal angle \(\phi = 2\pi - \theta_p\), and is inside the Bloch sphere of radius \(N/2\) — another indicator of fragmentation. For \textit{any} unfragmented state is a coherent state |\(\theta, \chi\rangle\rangle\) and the Bloch vector \textit{always} lies on the Bloch sphere, the orientation being given by polar angle \(\pi - 2\theta\) and azimuthal angle \(2\pi - \chi\). Thus \textit{any} state for which the Bloch vector lies inside the Bloch sphere must be a fragmented state, and the relative phase eigenstate is such a case.

Spin operators along (\(\hat{J}_z\)) and perpendicular (\(\hat{J}_x, \hat{J}_y\)) to the Bloch vector may be defined by

\[
\hat{J}_x = \hat{S}_x \\
\hat{J}_y = \hat{S}_x \sin \theta_p + \hat{S}_y \cos \theta_p \\
\hat{J}_z = \hat{S}_x \cos \theta_p - \hat{S}_y \sin \theta_p
\]

and in terms of the new spin operators

\[
\langle \hat{J}_x \rangle = 0 \\
\langle \hat{J}_y \rangle = 0 \\
\langle \hat{J}_z \rangle = \frac{\pi}{8} N \approx 0.392N
\]

The covariance matrix (see Appendix) which describes the quantum fluctuations for the spin operator components can be shown to be diagonal for the new spin operators \(\hat{J}_x, \hat{J}_y, \hat{J}_z\). For large \(N\) the fluctuations in the new Bloch vector components for the relative phase eigenstate are found to be (see Appendix)

\[
\delta \hat{J}_x \approx \sqrt{1/2} N \approx 0.289N \\
\delta \hat{J}_y \approx \sqrt{1/8 + 1/4 \ln N} \\
\delta \hat{J}_z \approx \sqrt{1/(6 - \pi^2/64)}N \approx 0.112N
\]

where \(\delta \hat{\Omega}^2 \equiv \langle (\hat{\Omega} - \langle \hat{\Omega} \rangle)^2 \rangle\). As \(| \langle \hat{J}_z \rangle \rangle/2 \approx 0.196N\) we see that for all \(N > 4\) the product \(\delta \hat{J}_x \cdot \delta \hat{J}_y > 0.198N\), which is greater than \(| \langle \hat{J}_z \rangle \rangle/2 \) consistent with
the Heisenberg uncertainty principle. However, although $\hat{J}_x$ is not squeezed, the other perpendicular component $\hat{J}_y$ is highly squeezed, with a fractional fluctuation $\delta \hat{J}_y / \langle \hat{J}_x \rangle$ essentially of order $1/N$ due to the denominator $\langle \hat{J}_x \rangle$. The numerator $\delta \hat{J}_y$ is a very slowly increasing function of $N$ - for $N$ changing from $10^8$ to $10^{10}$ it only changes from 2.17 to 2.42. The relative phase state could be of interest in Heisenberg limited interferometry \[25\]. By contrast, the fluctuations in the Bloch vector components for the coherent state $|\theta, \chi \rangle$ are $\delta \hat{J}_x \approx \sqrt{N}$, $\delta \hat{J}_y \approx \sqrt{N}$ and $\delta \hat{J}_z \approx 0$. Here the fluctuations are equal for the two components perpendicular to the Bloch vector, so there is no squeezing. Furthermore, the fractional fluctuation $\delta \hat{J}_{x,y} / \langle \hat{J}_z \rangle$ is only of order $1/\sqrt{N}$, corresponding to the standard quantum limit and not to the Heisenberg limit, as is the case for the relative phase eigenstate.

4 Applications of relative phase eigenstates

The relative phase eigenstate provides a useful theoretical concept for describing interferometry experiments based on BEC. This type of application is discussed in this Section, firstly in general terms and then for a specific BEC interferometry proposal. However, before treating these applications the question of whether the relative phase eigenstate can be prepared via some sort of dynamical process will be examined.

4.1 Creating relative phase eigenstates

The energy and energy fluctuation associated with the relative phase eigenstate are quite large. The typical two mode system such as bosons in a double well potential is described via the Josephson Hamiltonian

$$\hat{H} = -J \hat{S}_x + \delta \hat{S}_z + U \hat{S}_z^2$$

where $J$ is the inter-well tunneling parameter, $\delta$ describes asymmetry of the two wells and $U$ is the collision parameter. It is easy to see that the relative phase state (1) is not an energy eigenstate. The non-zero matrix elements of the Josephson Hamiltonian between the basis states $|N/2, k \rangle \equiv |N/2 - k \rangle_{a} |N/2 + k \rangle_{b}$ are

$$H_{k,k} = \delta k + Uk^2$$

$$H_{k,k+1} = -J \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - (k + 1)k}$$

$$H_{k,k-1} = -J \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - (k - 1)k}$$

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and for the relative phase state to be an energy eigenstate with energy $E$ requires

$$E = \delta k + U k^2 - \frac{J}{2} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right)} - (k + 1) k \exp(+i\theta_p)$$

$$- \frac{J}{2} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right)} - (k - 1) k \exp(-i\theta_p)$$

(21)

for all $k$, which is not possible. The mean energy $\langle \hat{H} \rangle$ is

$$\langle \hat{H} \rangle = U \frac{1}{12} N^2 - J \cos \theta_p \frac{\pi}{8} N$$

(22)

so in the Rabi regime [20] where $J \gg U N$ the mean energy is approximately $-J \cos \theta_p \frac{\pi}{8} N$, whilst in the Fock regime [20] where $U \gg J N$ it is essentially $U \frac{1}{12} N^2$.

The variance in the energy $\delta \hat{H}^2 = \langle (\hat{H} - \langle \hat{H} \rangle)^2 \rangle$ is given by

$$\delta \hat{H}^2 = N^2 \times \left[ \begin{array}{ccc} U N & J & \delta \end{array} \right] \times \left[ \begin{array}{ccc} \frac{1}{12} & \cos \theta_p & 0 \\
\frac{\pi}{84} & 0 & 0 \\
0 & (\frac{1}{6} - \frac{\pi^2}{64}) \cos^2 \theta_p & \frac{1}{12} \end{array} \right] \times \left[ \begin{array}{c} U N \\
J \\
\delta \end{array} \right]$$

(23)

correct to $O(N^2)$ (see Appendix for details). This is a quadratic form in the quantities $U N$, $J$, and $\delta$. That this form is positive definite can be shown by determining the eigenvalues $\lambda_1(\theta_p)$, $\lambda_2(\theta_p)$ and $\lambda_3(\theta_p)$ of the 3x3 matrix in Eq.(23), and explicit formulae are given in the Appendix. As expected the eigenvalues are all real and positive for all relative phase $\theta_p$ (see Figure A in Appendix). It is of some interest to consider cases where the Josephson parameters are related via

$$\left[ \begin{array}{c} U N \\
J \\
\delta \end{array} \right] = K \left[ \begin{array}{c} X_{1\alpha} \\
X_{2\alpha} \\
X_{3\alpha} \end{array} \right]$$

(24)

where $\left[ \begin{array}{ccc} X_{1\alpha} & X_{2\alpha} & X_{3\alpha} \end{array} \right]^T$ are the orthonormal column eigenvectors associated with the eigenvalues $\lambda_1(\theta_p)$, $\lambda_2(\theta_p)$ and $\lambda_3(\theta_p)$ and $K$ is arbitrary. In this case an expression for the relative energy fluctuation can be obtained as

$$\sqrt{\langle \delta \hat{H}^2 \rangle_\alpha} = \frac{\sqrt{\lambda_\alpha(\theta_p)}}{|(X_{1\alpha} \frac{1}{12} - X_{2\alpha} \cos \theta_p \frac{\pi}{8})|}$$

(25)

for the eigenvalues $\lambda_1(\theta_p)$, $\lambda_2(\theta_p)$. For $\lambda_3(\theta_p)$ we have $\langle \hat{H} \rangle = 0$, so the relative fluctuation is undefined. In Figures 1 and 2 the relative energy fluctuations are shown for $\lambda_1(\theta_p)$, $\lambda_2(\theta_p)$ respectively.
Clearly for the choice of Josephson parameters in the $\lambda_1(\theta_p)$ case the relative energy fluctuations are very large, $O(200\%)$. However, for the choice of Josephson parameters in the $\lambda_2(\theta_p)$ case the relative energy fluctuations are fairly small, $O(6\%)$. If the Josephson parameters are chosen as in the latter case, then an adiabatic process starting with parameters as for some initial $\theta_p$ and changing them to those for $\theta_p$ in accordance with Eq. (24) with $\alpha = 2$ could prepare a state close to the required relative phase state. For example, with $\theta_{p0} = \frac{\pi}{2}$ we have $UN = 0$, $J = K$ and $\delta = 0$ since $X_{12} = 0$, $X_{22} = 1$ and $X_{32} = 0$. A suitable initial state within the Rabi regime where $J \gg UN, \delta = 0$ might be used. In particular, the state discussed below corresponding to that created at the end of the first stage in the proposed Heisenberg limited interferometry experiment has a quite well defined relative phase $\theta_{p0} = 0$ (see Figure 4 below) and might be suitable. The required quantities $X_{12}$ and $X_{22}$ that define the way $UN, J$ would be adiabatically changed to reach any required $\theta_p$ are shown in Figure 3 (formulae are also given in the Appendix). $\delta$ would remain equal to zero.

Figure 3. Eigenvector for $\lambda_2(\theta_p)$. $X_{12}$ (blue curve) and $X_{22}$ (red curve). $X_{32} = 0$. 
No actual experiment for preparing a BEC in a relative phase eigenstate or for directly measuring the relative phase probability have yet been carried out, so the relative phase probability distribution may need to be inferred from other measurements rather than directly measured. However, similar remarks may be made about position eigenstates for individual particles - where only states with relatively localised positions can be prepared and where position probability results are inferred from experiments involving scattering of weak probe beams, so this need not preclude the relative phase operator and its eigenstates being useful concepts in quantum atom optics.

4.2 Interferometry experiments an quantum correlation functions

The quantum correlation function $G^{(1)}(r, r')$ with $r = r'$ is of particular interest as it determines the probability distribution for boson position measurements \[29], \[30] and hence is useful in describing the interference fringes that can occur in BEC interferometry experiments. For a general state the first order quantum correlation function can also be expressed in terms of the amplitudes $A(\theta_p)$ for the relative phase eigenstates. These amplitudes appear via three autocorrelation functions. We have

$$G^{(1)}(r, r') = \phi_a(r)^* \phi_a(r') \sum_r C_0(\theta_r) \frac{1}{N+1} \sum_k \exp(ik\theta_r) \left( \frac{N}{2} - k \right) + \phi_b(r)^* \phi_b(r') \sum_r C_0(\theta_r) \frac{1}{N+1} \sum_k \exp(ik\theta_r) \left( \frac{N}{2} + k \right) + \phi_a(r)^* \phi_b(r') \sum_r C_{+1}(\theta_r) \frac{1}{N+1} \sum_k \exp(ik\theta_r) \sqrt{\left( \frac{N}{2} - k + 1 \right) \left( \frac{N}{2} + k \right)} + \phi_b(r)^* \phi_a(r') \sum_r C_{-1}(\theta_r) \frac{1}{N+1} \sum_k \exp(ik\theta_r) \sqrt{\left( \frac{N}{2} + k + 1 \right) \left( \frac{N}{2} - k \right)}$$

(26)

where the autocorrelation functions of the amplitudes $A(\theta_p)$ are defined as

$$C_0(\theta_r) = \sum_{q=-N}^{N} A(\{\theta_r + \theta_q\}_{\mod 2\pi}) A(\theta_q)^*$$

$$C_{\pm 1}(\theta_r) = \sum_{q=-N}^{N} A(\{\theta_r + \theta_q\}_{\mod 2\pi}) A(\theta_q)^* \exp(\pm i\theta_q)$$

(27)

Hence we see that for a state with a relative narrow relative phase distribution around a particular phase $\theta_0$ ($A(\theta_p) \approx \delta_{\theta_p, \theta_0}$) the autocorrelation function $C_0(\theta_r)$ will be peaked around $\theta_r \approx 0$, whilst the autocorrelation functions
\[ C_{\pm 1}(\theta_r) \] will be peaked around \( \theta_r = \mp \theta_0 \). This means that the first two terms in \( G^{(1)}(r, r') \) have no dependence on \( \theta_0 \), whereas the last two terms have essentially a sinusoidal variation with \( \theta_0 \) since the sum over \( \theta_r \) will be dominated by terms \( \theta_r = \mp \theta_0 \). If the particular central phase \( \theta_0 \) is changed during an experiment then the boson position probability will change - hence a fringe pattern would be observed. Note that the observation of the fringe depends on the overlap of the mode functions being sufficiently large. On the other, for a state with a relatively wide relative phase distribution the auto correlation functions will be significant for a wide range of \( \theta_r \) so the sum over \( \theta_r \) will be no longer be dominated by terms \( \theta_r = \mp \theta_0 \) and the fringe pattern would be washed out.

4.3 Heisenberg limited BEC interferometry experiment

The relative phase eigenstate is a valuable theoretical concept for describing the behaviour in BEC interferometry experiments. For example, in the proposed experiment by Dunningham and Burnett \[31\] for Heisenberg limited interferometry in two mode BEC, the collapse and revival of interference fringes can be discussed in terms of collapses and revivals of the time dependent probability distribution for the relative phase. Collapse and revival effects in BEC were described earlier by Wright et al \[32\].

The Dunningham and Burnett experiment treats the two mode double well BEC system via the Josephson Hamiltonian. The experiment has two stages. In the first stage the system starts with equal numbers of bosons in each well, so the quantum state is \( |\Phi(0)\rangle = |N/2\rangle_a |N/2\rangle_b \), so \( b_k(0) = \delta_{k,0} \). From Eqs. (4) and (6) it is easy to see that the relative phase probability distribution is uniform. With evolution dominated by the tunneling term the state evolves for a time \( T_1 = \pi/2 \) (or when \( \phi = Jt/\hbar = \pi/2 \)) The methods of angular momentum theory can be used to determine the dynamics, since the evolution operator \( \hat{U}(t) = \exp(i\hat{S}_x Jt/\hbar) \) is just a rotation operator. We find that

\[
\begin{align*}
  b_k(T_1) &= \exp(ik\pi/2) \sqrt{(N/2 + k)!(N/2 - k)!/(N/2)!(2^{N/2})} \sum_p (-1)^p C_{p+k}^{N/2} C_p^{N/2} 
\end{align*}
\]

from which we can calculate the relative phase probability distribution via Eqs. (4) and (6). This is shown in Figure 4 for the case \( N = 80 \) and we see that the system has a well-defined relative phase of approximately zero. This stage of the experiment involves creating a state with a rather well-defined relative phase. Experimentally the time \( T_1 \) is determined by observing the time it takes for the fringe pattern to become sharpest.

Figure 4. Relative phase probability at end of the first stage. Well defined relative phase seen. Parameters are given in text.
The second stage involves evolution for a further time $T$ dominated by the collision term, or the collision term plus the asymmetry term. In this case we find that

$$b_k(T_1 + T) = \exp(-ik\frac{\delta T}{\hbar})\exp(-ik^2\frac{UT}{\hbar})b_k(T_1)$$

We first consider the situation when there is no asymmetry $\delta = 0$. A characteristic time scale for the collision dominated evolution is $T_2 = \pi \hbar / 2U$ (or when $\xi = Ut/\hbar = \pi/2$). However, due to the $\exp(-ik^2UT/\hbar)$ factor there is a dephasing effect, causing the relative phase probability amplitudes $A(\theta_p, T_1 + T)$ to become significant over a wide range of $\theta_p$. This causes a collapse in the previously well defined interference fringe pattern. The time scale for this to happen is that required for the fastest pairs of contributions ($k = -N/2, -N/2 + 1$ or $k = +N/2, +N/2 - 1$) to get out of phase by $\sim \pi$. Thus the collapse time is given by $T_c = \pi \hbar / NU = T_2/N$ (or when $\xi = \pi/2N$), which is $O(1/N)$ times shorter than $T_2$. This collapse effect is shown in Figures 5 and 6 for $N = 80$. For $\xi = 0.001\pi$ the relative phase distribution is starting to spread out and is essentially uniform when $\xi = 0.01\pi$.

Figure 5. Relative phase probability just after the end of the first stage. Dephasing effects starting to be seen. Parameters are given in text.

Figure 6. Relative phase probability somewhat after the end of the first stage. Complete dephasing effects seen. Parameters are given in text.
Prob Phase Q for Phi = Pi/2 and Xi = 0.001 Pi

Prob Phase Q for Phi = Pi/2 and Xi = 0.01 Pi
However, the factors $\exp(-i k^2 U t/\hbar)$ do eventually get back into phase. If $\xi = U t/\hbar$ is a multiple of $\pi/2$ then all the phase factors have a modulus of unity, irrespective of $k$. Hence a revival of the relative phase probability distribution to the sharply defined distribution that occurred at the end of the first stage will take place. The revival time scale is thus given by $T_{rev} = T_2 = \pi \hbar/2U$ (or when $\xi = U t/\hbar = \pi/2$). This is shown in Figure 7 for $N = 80$. In Figure 8 the time is slightly longer than $T_{rev}$ and the relative phase distribution is starting to collapse again.

Figure 7. Relative phase probability at the end of the second stage. Revival of well-defined phase seen. Parameters are given in text.

Figure 8. Relative phase probability just after the end of the second stage. Beginning of collapse of well-defined phase seen. Parameters are given in text.

We now consider the effect of asymmetry. It is easy to see that at time $T_1 + T_2$ the relative phase amplitude for non zero $\delta$ is given by

$$A(\theta_p, T_1 + T_2) = A(\theta_p + \delta T_2/\hbar, T_1 + T_2)_{\delta=0}$$

so is of the same form as when there is no asymmetry, but with the relative phase shifted by $\delta T_2/\hbar = (\delta/U)\pi/2$. This effect is shown in Figure 9 for $N = 80$. The shift in the fringe pattern would be observable if $\delta$ is a reasonable fraction of $U$.  


Prob Phase Q for Phi = Pi/2 and Xi = 0.501 Pi

Prob Phase Q for Phi = Pi/2, Xi = 0.5 Pi and Asym = 0.2 Pi
Evolution during the second stage of the experiment is allowed to occur for a time $T_2$ corresponding to the revival time, and with zero asymmetry present. The revival time could be determined experimentally by observing when the sharp fringes obtained at the end of the first stage are restored again. The accuracy in determining the revival time is given by the collapse time, so the fractional error in the revival time $T_{rev}$ is of order $1/N$. If the second stage is run again with asymmetry present the fringe pattern at the revival time is shifted by $\delta T_{rev}/\hbar$. If this phase shift is measured with perfect accuracy, then the fractional error in measuring $\delta$ is the same as that for $T_{rev}$, and hence is of order $1/N$. This represents a Heisenberg limited interferometry measurement of the asymmetry, scaling as the inverse of the total number of bosons.

5 Summary

This paper presents an approach to treating phase in quantum atom optics in which phase is regarded as a physical quantity for the system and treated theoretically as a linear Hermitian operator, similar to the Pegg-Barnett treatment of phase in quantum optics. Other approaches to treating phase are discussed and a brief review outlines previous attempts to find a Hermitian phase operator. The Pegg-Barnett approach is adapted to define a relative phase operator for two mode systems via first introducing a complete orthonormal set of relative phase eigenstates. These states are contrasted with other so-called phase states. The entanglement, fragmentation and spin squeezing properties of the relative phase states are set out. The relative phase state has maximal two mode entanglement, it is a fragmented state with its Bloch vector lying inside the Bloch sphere and is highly spin squeezed. In the final section applications of the relative phase states in describing BEC interferometry experiments are made, both in general and in the context of a proposed Heisenberg limited interferometry experiment. Interferometry experiments essentially measure the autocorrelation functions for the relative phase amplitudes. The possibility for preparing a BEC in a relative phase state is examined, and an approach based on adiabatically changing parameters in the Josephson Hamiltonian is suggested. However, the difficulty is similar to preparing a particle system in a position eigenstate. In spite of this, the relative phase states are still a useful concept for describing experiments in quantum atom optics. Finally, if such a highly spin squeezed state could be prepared it may be useful for Heisenberg limited interferometry in view of the fractional fluctuation in one of the spin operator components perpendicular to the Bloch vector being essentially only of order $1/N$. 

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7 Appendix

In the appendix we summarize certain key results needed in the main body of the paper.

7.1 Field operators

For the two mode BEC the field operators are given in the two mode approximation as

\[ \hat{\Psi}(r) = \hat{a}\phi_a(r) + \hat{b}\phi_b(r) \]

and with the usual non-zero commutation rules for the mode operators \( [\hat{a}, \hat{a}^\dagger] = [\hat{b}, \hat{b}^\dagger] = 1 \), the non-zero commutation rule for the field operators is

\[ [\hat{\Psi}(r), \hat{\Psi}(r')^\dagger] = \phi_a(r)\phi_a^*(r') + \phi_b(r)\phi_b^*(r') = \delta_2(r, r') \]

which is a restricted delta function for the space spanned by the two orthonormal mode functions.

7.2 Spin operators and spin states

Because of the two-mode approximation it is possible to treat the bosonic system using the methods of angular momentum theory. The system behaves like a macroscopic spin system with angular momentum quantum number \( j = \frac{N}{2} \).

In a two-mode theory it is convenient to introduce the Schwinger spin angular momentum operators defined by

\[ \hat{S}_x = (\hat{b}^\dagger\hat{a} + \hat{a}^\dagger\hat{b})/2 \]
\[ \hat{S}_y = (\hat{b}^\dagger\hat{a} - \hat{a}^\dagger\hat{b})/2i \]
\[ \hat{S}_z = (\hat{b}^\dagger\hat{b} - \hat{a}^\dagger\hat{a})/2 \]

The spin operators \( \hat{S}_a \) satisfy the standard commutation rules for angular momentum operators

\[ [\hat{S}_a, \hat{S}_b] = i\epsilon_{abc}\hat{S}_c \quad (a, b, c = x, y, z), \]

and the square of the angular momentum \( (\hat{S})^2 \) can be related to the boson number operator. Thus:

\[ (\hat{S})^2 = \sum_a (\hat{S}_a)^2 \]
\[ = \frac{\hat{N}}{2}(\frac{\hat{N}}{2} + 1) \]

23
where
\[ \hat{N} = (\hat{b}^\dagger \hat{b} + \hat{a}^\dagger \hat{a}) \]  
(34)
is the number operator. Clearly the angular momentum squared is a conserved quantity. Note that the spin operator \( \hat{S}_z \) is the same as the relative number operator \( \delta \hat{N} \).

The \( N \) boson system behaves like a giant spin system in the two-mode approximation. The basis states \( |N/2-k\rangle_a |N/2+k\rangle_b \) are simultaneous eigenstates of \( (\hat{S}_z)^2 \) and \( \hat{S}_z \) with eigenvalues \( N^2 (N^2 + 1) \) and \( k \) respectively. To emphasize the spin character of the basis states we can introduce the notation
\[ |N/2-k\rangle_a |N/2+k\rangle_b \equiv \left( \hat{a}^\dagger \right)^{\frac{N-k}{2}} \left( \hat{b}^\dagger \right)^{\frac{N+k}{2}} |0\rangle \]
(35)

Thus:
\[ (\hat{S}_z)^2 |N/2,k\rangle = N^2 \left( \frac{N}{2} + 1 \right) |N/2,k\rangle \]
(36)
\[ \hat{S}_z |N/2,k\rangle = k \left( \frac{N}{2} \right) \]
(37)

Hence \( j = \frac{N}{2} \) is the spin angular momentum quantum number, and \( k \) is the spin magnetic quantum number, with \( -\frac{N}{2} \leq k \leq \frac{N}{2} \). Thus the boson number \( N \) and the quantity \( k \) that specifies the fragmentation of the BEC between the two modes have a physical interpretation in terms of angular momentum theory. Since boson numbers may be \( \sim 10^8 \) the spin system is on a macroscopic scale.

As in angular momentum theory we find it convenient to introduce spin up \( \hat{S}_+ \) and spin down \( \hat{S}_- \) operators, which change the spin magnetic quantum numbers by \( \pm 1 \). We have
\[ \hat{S}_\pm \left| \frac{N}{2}, k \right\rangle = \left\{ \frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k \pm 1) \right\}^{\frac{1}{2}} \left| \frac{N}{2}, k \pm 1 \right\rangle \]
\[ = \left\{ \frac{N}{2} \mp k \left( \frac{N}{2} \pm k + 1 \right) \right\}^{\frac{1}{2}} \left| \frac{N}{2}, k \pm 1 \right\rangle \]
(38)

The methods of angular momentum theory can be utilized by first writing the full Hamiltonian in terms of spin operators using equations (29), (31), (34) - noting that all terms involve equal numbers of creation and annihilation operators, and its matrix elements calculated using angular momentum theory from (37) and (38). The same applies in a simplification to the full Hamiltonian giving rise to the Josephson Hamiltonian.
7.3 Quantum correlation functions

The first order quantum correlation function is defined as

$$G^{(1)}(\mathbf{r}, \mathbf{r}') = \langle \hat{\Psi}(\mathbf{r})^\dagger \hat{\Psi}(\mathbf{r}') \rangle$$  \hspace{1cm} (39)$$

and for the pure state given by (5) this is found to be

$$G^{(1)}(\mathbf{r}, \mathbf{r}') = \sum_k b_k^* b_{k+1} \left\{ \phi_a(\mathbf{r})^* \phi_a(\mathbf{r}') \left( \frac{N}{2} + k \right) + \phi_b(\mathbf{r})^* \phi_b(\mathbf{r}') \left( \frac{N}{2} + k + 1 \right) \right\}$$

$$+ \sum_k b_k^* b_{k+1} \left\{ \phi_b(\mathbf{r})^* \phi_a(\mathbf{r}') \left( \frac{N}{2} + k \right) + \phi_a(\mathbf{r})^* \phi_b(\mathbf{r}') \left( \frac{N}{2} + k + 1 \right) \right\}$$  \hspace{1cm} (40)$$

7.4 Bloch vector

The components $S_a$ of the Bloch vector are given by averages of the spin operators $\hat{S}_a$

$$S_a = \langle \hat{S}_a \rangle \hspace{1cm} (a = x, y, z)$$  \hspace{1cm} (41)$$

Often the Bloch vector components are scaled in units of $N$, but to avoid extra notation we will not do that here.

Since $\hat{S}_a$ is hermitian and $\langle \hat{S}_a^2 \rangle \leq \langle (\hat{S}_a)^2 \rangle$ and using (33) we see that

$$0 \leq \sum_a S_a^2 \leq \sum_a \langle \hat{S}_a^2 \rangle = \frac{N}{2} \left( \frac{N}{2} + 1 \right) = \frac{N^2}{4} \hspace{1cm} N \gg 1$$  \hspace{1cm} (42)$$

showing that for all states the Bloch vector lies inside or on a Bloch sphere, whose radius is $\frac{N}{2}$.

For the quantum state given by (5) expressions for the Bloch vector components are

$$S_\pm = \sum_k b_k^* b_{k+1} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k \mp 1)}$$

$$S_x = (S_+ + S_-)/2 \hspace{1cm} S_y = (S_+ - S_-)/2i$$

$$S_z = \sum_k b_k^* b_k k$$  \hspace{1cm} (43)$$

and these are related to the first order quantum correlation function via

$$G^{(1)}(\mathbf{r}, \mathbf{r}') = \left( \begin{array}{c}
\frac{N}{2} \left\{ \phi_a(\mathbf{r})^* \phi_a(\mathbf{r}') + \phi_b(\mathbf{r})^* \phi_b(\mathbf{r}') \right\} \\
+S_z \left\{ -\phi_a(\mathbf{r})^* \phi_a(\mathbf{r}') + \phi_b(\mathbf{r})^* \phi_b(\mathbf{r}') \right\} \\
+S_- \{ \phi_a(\mathbf{r})^* \phi_b(\mathbf{r}') \} + S_+ \{ \phi_b(\mathbf{r})^* \phi_a(\mathbf{r}') \}
\end{array} \right)$$  \hspace{1cm} (44)$$
7.5 Covariance matrix for spin operators

The covariance matrix $C(\hat{S}_a, \hat{S}_b)$ for the spin operators $\hat{S}_a$ is given by

$$C(\hat{S}_a, \hat{S}_b) = \frac{1}{2} \left( \langle \Delta \hat{S}_a \Delta \hat{S}_b \rangle + \langle \Delta \hat{S}_b \Delta \hat{S}_a \rangle \right)$$ (45)

$$\Delta \hat{S}_a = \hat{S}_a - \left\langle \hat{S}_a \right\rangle$$ (46)

where $\Delta \hat{S}_a$ is a spin fluctuation operator. It is easy to see that the $3 \times 3$ covariance matrix is real and symmetric and that $C(\hat{S}_a, \hat{S}_a)$ gives the variance $\langle (\Delta \hat{S}_a)^2 \rangle$ for $\hat{S}_a$. These are the square of the standard deviations or fluctuations. Such a matrix defines a positive quadratic form $F(\xi_x, \xi_y, \xi_z)$. With real $\xi_a$ we have

$$F(\xi_x, \xi_y, \xi_z) = \sum_{a,b} \xi_a C(\hat{S}_a, \hat{S}_b) \xi_b$$

$$= \frac{1}{2} \left( \sum_a \xi_a \Delta \hat{S}_a \sum_b \xi_b \Delta \hat{S}_b \right) + \left( \sum_b \xi_b \Delta \hat{S}_b \sum_a \xi_a \Delta \hat{S}_a \right)$$

$$= \left\langle S(\xi)^\dagger S(\xi) \right\rangle \geq 0$$ (47)

for any state, where $S(\xi) = \sum_a \xi_a \Delta \hat{S}_a = S(\xi)^\dagger$. Hence the three eigenvalues for the covariance matrix will be real and positive. Linear combinations of the $\Delta \hat{S}_a$ involving a real orthogonal matrix will diagonalise the covariance matrix and the diagonal elements will give the variances for fluctuations in three orthogonal directions. These specify the principal quantum fluctuations.

The covariance matrix can also be written as

$$C(\hat{S}_a, \hat{S}_b) = \frac{1}{2} \left( \left\langle \hat{S}_a \hat{S}_b + \hat{S}_b \hat{S}_a \right\rangle - \left\langle \hat{S}_a \right\rangle \left\langle \hat{S}_b \right\rangle \right)$$ (48)

so it measures the difference between the average of half the anti-commutator of $\hat{S}_a, \hat{S}_b$ and the product of the averages of the separate $\hat{S}_a, \hat{S}_b$.

Expressions for the covariance matrix elements for the spin operators in the
case of the pure state given by (5) are as follows.

\[
C_{xx} = C(\hat{S}_x, \hat{S}_x) \\
= \frac{1}{4} \sum_k b_k^* b_{k+2} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k+1)} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - (k+1)(k+2)} \\
+ \frac{1}{2} \sum_k b_k^* b_k \left( \frac{N}{2} \left( \frac{N}{2} + 1 \right) - k^2 \right) \\
+ \frac{1}{4} \sum_k b_k^* b_{k-2} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k-1)} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - (k-1)(k-2)} \\
- \frac{1}{4} \left( \sum_k b_{k+1}^* b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k+1)} - \sum_k b_{k-1}^* b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k-1)} \right)^2
\]

(49)

and

\[
C_{xy} = C(\hat{S}_x, \hat{S}_y) = C_{yx} \\
= \frac{1}{4i} \sum_k b_k^* b_{k+2} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k+1)} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - (k+1)(k+2)} \\
- \frac{1}{4i} \sum_k b_k^* b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k-1)} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - (k-1)(k-2)} \\
- \frac{1}{4i} \left( \sum_k b_{k+1}^* b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k+1)} \right)^2 \\
+ \frac{1}{4i} \left( \sum_k b_{k-1}^* b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k-1)} \right)^2
\]

(50)
and

\[ C_{xx} = C(\hat{S}_x, \hat{S}_z) = C_{zx} \]
\[ = \frac{1}{4} \sum_k b_{k+1}^* b_k (2k + 1) \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k + 1)} \]
\[ + \frac{1}{4} \sum_k b_{k-1}^* b_k (2k - 1) \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k - 1)} \]
\[ - \frac{1}{2} \sum_k b_{k+1}^* b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k + 1)} \sum_k b_k^* b_k k \] (51)

and

\[ C_{yy} = C(\hat{S}_y, \hat{S}_y) \]
\[ = -\frac{1}{4} \sum_k b_{k+2}^* b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k + 1)} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - (k + 1)(k + 2)} \]
\[ + \frac{1}{2} \sum_k b_k^* b_k \left( \frac{N}{2} \left( \frac{N}{2} + 1 \right) - k^2 \right) \]
\[ - \frac{1}{4} \sum_k b_{k-2}^* b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k - 1)} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - (k - 1)(k - 2)} \]
\[ + \frac{1}{4} \left( \sum_k b_{k+1}^* b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k + 1)} \right)^2 \]
\[ - \sum_k b_{k-1}^* b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k - 1)} \] (52)
and

\[ C_{yz} = C(\hat{S}_y, \hat{S}_z) = C_{zy} \]
\[ = \frac{1}{4i} \sum_k b_k^{*} b_{k+1} (2k+1) \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k+1)} \]
\[ - \frac{1}{4i} \sum_k b_k^{*} b_{k-1} (2k-1) \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k-1)} \]
\[ - \frac{1}{2i} \sum_k b_k^{*} b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k+1)} \sum_k b_k^{*} b_k k \]
\[ + \frac{1}{2i} \sum_k b_k^{*} b_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k-1)} \sum_k b_k^{*} b_k k \]  \hspace{1cm} (53)

and finally

\[ C_{zz} = C(\hat{S}_z, \hat{S}_z) \]
\[ = \sum_k b_k^{*} b_k k^2 - \left( \sum_k b_k^{*} b_k k \right)^2 \]  \hspace{1cm} (54)

In terms of the new spin operators defined via the orthogonal transformation in (16), the new covariance matrix is given by

\[ C(\hat{J}_a, \hat{J}_b) = \sum_{c,d} M_{ac}(\theta_p) C(\hat{S}_c, \hat{S}_d) M_{bd}(\theta_p) = \delta_{ab} \left\langle (\Delta \hat{J}_a)^2 \right\rangle \]  \hspace{1cm} (55)

where

\[ [M(\theta_p)] = \begin{bmatrix} 0 & 0 & 1 \\ \sin \theta_p & \cos \theta_p & 0 \\ \cos \theta_p & -\sin \theta_p & 0 \end{bmatrix} \]  \hspace{1cm} (56)

relates the new and original spin operators via

\[ \hat{J}_a = \sum_c M_{ac}(\theta_p) \hat{S}_c \]  \hspace{1cm} (57)

It turns out that the new covariance matrix is diagonal. The evaluation of the original covariance matrix involves the following sums for \( N \) large:

\[ (a) \sum_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k \pm 1)/(N+1)} \div \frac{\pi N}{8} \]
\[ (b) \sum_k \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - k(k \pm 1)} \sqrt{\frac{N}{2} \left( \frac{N}{2} + 1 \right) - (k \pm 1)(k \pm 2)/(N+1)} \div \frac{\pi^2}{6} \]
\[ (c) \sum_k \frac{\sqrt{N/2}}{N+1} \div \frac{\pi^2}{6} \]
These sums are correct to $O(N)$. This gives the new covariance matrix to $O(N)$ as

$$\begin{bmatrix} C(\hat{J}_a, \hat{J}_b) \end{bmatrix} = \begin{bmatrix} (\frac{1}{12}) N^2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \left(\frac{1}{8} - \frac{\pi^2}{64}\right) N^2 \end{bmatrix}$$

(58)

showing that correct to $O(N)$ the variances for $\hat{J}_x, \hat{J}_z$ are large but that for $\hat{J}_y$ is zero.

To determine the new covariance matrix more accurately we begin again with the new spin operators still given by (57) and work out the expressions for $C(\hat{J}_a, \hat{J}_b)$ to $O(N^0)$ when the term is zero correct to $O(N)$. As before we find the new covariance matrix is diagonal but now given by

$$\begin{bmatrix} C(\hat{J}_a, \hat{J}_b) \end{bmatrix} = \begin{bmatrix} (\frac{1}{12}) N^2 & 0 & 0 \\ 0 & \frac{1}{8} + \frac{1}{4} \ln N & 0 \\ 0 & 0 & \left(\frac{1}{8} - \frac{\pi^2}{64}\right) N^2 \end{bmatrix}$$

(59)

The new variance for $\hat{J}_y$ is now found to be non-zero and given by $\frac{1}{8} + \frac{1}{4} \ln N$. This requires the following sum:

$$(e) \sum_c \left(\sqrt{\frac{\pi}{2} (\frac{\pi}{2} + 1) - k(k + 1)} \right) \sqrt{\frac{\pi}{2} (\frac{\pi}{2} + 1) - (k + 1)(k + 2)/2(N+1) + \sum_c \left(\sqrt{\frac{\pi}{2} (\frac{\pi}{2} + 1) - k(k + 1)} \right)} / 2(N+1) \right) \equiv \frac{1}{8} + \frac{1}{4} \ln N.$$

7.6 Energy fluctuations

The Josephson Hamiltonian is given by

$$\hat{H} = U \hat{S}_z^2 - J \hat{S}_x + \delta \hat{S}_x$$

(60)

and it is straightforward to show that then variance in the energy is given by

$$\delta \hat{H}^2 = \begin{bmatrix} U & -J & \delta \\ -J & 0 & 0 \\ \delta & 0 & 0 \end{bmatrix} \times \begin{bmatrix} \{\hat{S}_x, \hat{S}_x^2\} & \{\hat{S}_z, \hat{S}_x^2\} & \{\hat{S}_z, \hat{S}_z\} \\ \{\hat{S}_x, \hat{S}_x^2\} & \{\hat{S}_x, \hat{S}_z\} & \{\hat{S}_z, \hat{S}_z\} \\ \{\hat{S}_z, \hat{S}_x^2\} & \{\hat{S}_z, \hat{S}_z\} & \{\hat{S}_z, \hat{S}_z\} \end{bmatrix} \times \begin{bmatrix} U \\ -J \\ \delta \end{bmatrix}$$

(61)

which involves the covariances of $\hat{S}_x^2, \hat{S}_x$ and $\hat{S}_z$. Evaluating the covariances using certain sums given in the previous section plus

$$(f) \sum_k k^2/(N+1) \equiv \frac{N^2}{12}$$

$$(g) \sum_k k^4/(N+1) \equiv \frac{N^4}{90}$$

$$(h) \sum_k k(k+1) \sqrt{\frac{\pi}{2} (\frac{\pi}{2} + 1) - k(k + 1)/(N+1) \equiv \frac{\pi N^3}{128}}$$

we have correct to
\[ O(N^2) \]

\[ \delta \hat{H}^2 \]

\[
\begin{bmatrix}
U & -J & \delta \\
0 & \frac{\pi}{384} N^3 \cos \theta_p & (\frac{1}{6} - \frac{\pi^2}{64}) N^2 \cos^2 \theta_p & 0 \\
0 & 0 & \frac{\pi}{384} N^2 \cos \theta_p & 0 \\
\end{bmatrix}
\times
\begin{bmatrix}
U \\
-J \\
\delta \\
\end{bmatrix}
\]

\[
N^2 \times \begin{bmatrix}
U & N & J \\
0 & \frac{\pi}{384} N^3 \cos \theta_p & (\frac{1}{6} - \frac{\pi^2}{64}) N^2 \cos^2 \theta_p & 0 \\
0 & 0 & \frac{\pi}{384} N^2 \cos \theta_p & 0 \\
\end{bmatrix}
\times
\begin{bmatrix}
U \\
J \\
\delta \\
\end{bmatrix}
\]

which is a quadratic form in the quantities \( UN, J \) and \( \delta \). That this form is positive definite can be shown by determining the eigenvalues \( \lambda_1(\theta_p) \), \( \lambda_2(\theta_p) \) and \( \lambda_3(\theta_p) \) of the 3x3 matrix.

The corresponding eigenvalue equations are

\[
\begin{bmatrix}
\frac{1}{180} N^4 & -\frac{\pi}{384} N^3 \cos \theta_p & \frac{\pi}{384} N^3 \cos \theta_p & 0 \\
\frac{\pi}{384} N^2 \cos \theta_p & \frac{\pi}{384} N^2 \cos \theta_p & 0 & 0 \\
0 & 0 & \frac{1}{12} N^2 & 0 \\
\end{bmatrix}
\times
\begin{bmatrix}
X_{1\alpha} \\
X_{2\alpha} \\
X_{3\alpha} \\
\end{bmatrix}
= \lambda_\alpha(\theta_p)
\begin{bmatrix}
X_{1\alpha} \\
X_{2\alpha} \\
X_{3\alpha} \\
\end{bmatrix}
\]

where the eigenvectors are orthogonal and normalised to unity \( \sum_i X_{i\alpha} X_{i\beta} = \delta_{\alpha\beta} \). The eigenvalues are easily obtained as

\[
\begin{align*}
\lambda_1(\theta_p) &= \frac{1}{2} \left( (a + b) + \sqrt{(a - b)^2 + 4c^2} \right) \\
\lambda_2(\theta_p) &= \frac{1}{2} \left( (a + b) - \sqrt{(a - b)^2 + 4c^2} \right) \\
\lambda_3(\theta_p) &= d
\end{align*}
\]

with \( a = \frac{1}{180} \), \( b = (\frac{1}{6} - \frac{\pi^2}{64}) \cos^2 \theta_p \), \( c = \frac{\pi}{384} \cos \theta_p \) and \( d = \frac{1}{12} \). The eigenvalues are all real and positive, as may be seen in Figure 10 for the non-trivial \( \lambda_1(\theta_p) \), \( \lambda_2(\theta_p) \).

Figure 10. Eigenvalues \( \lambda_1(\theta_p) \) (blue curve) and \( \lambda_2(\theta_p) \) (red curve)
The corresponding eigenvectors are:

\[
\begin{bmatrix}
X_{11} \\
X_{21} \\
X_{31}
\end{bmatrix} = \frac{1}{\sqrt{(a-\lambda_1)^2 + c^2}} \begin{bmatrix}
-c \\
(a-\lambda_1) \\
0
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_{12} \\
X_{22} \\
X_{32}
\end{bmatrix} = \frac{1}{\sqrt{(a-\lambda_2)^2 + c^2}} \begin{bmatrix}
-c \\
(a-\lambda_2) \\
0
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_{13} \\
X_{23} \\
X_{33}
\end{bmatrix} = \begin{bmatrix}
0 \\
0 \\
1
\end{bmatrix}
\]

The eigenvector for \(\lambda_1(\theta_p)\) are shown in Figure 11.

Figure 11. Eigenvector for \(\lambda_1(\theta_p)\). \(X_{11}\) (blue curve) and \(X_{21}\) (red curve). \(X_{31} = 0\).

For the case where

\[
\begin{bmatrix}
UN \\
J \\
\delta
\end{bmatrix} = K \begin{bmatrix}
X_{1\alpha} \\
X_{2\alpha} \\
X_{3\alpha}
\end{bmatrix}
\]

(66)
where $K$ is arbitrary, it is easy to see that in this case the energy variance and standard deviation are given by

$$
\left\langle \delta \hat{H}^2 \right\rangle^\alpha_\alpha = N^2 K^2 \lambda_\alpha(\theta_p)
$$

$$
\sqrt{\left\langle \delta \hat{H}^2 \right\rangle^\alpha_\alpha} = NK \sqrt{\lambda_\alpha(\theta_p)} 
$$

(67)

The average energy in this case is

$$
\left\langle \hat{H} \right\rangle \doteq N \left( UN \frac{1}{12} - J \cos \theta_p \frac{\pi}{8} \right)
$$

$$
\left\langle \hat{H} \right\rangle_\alpha \doteq NK \left( X_{1\alpha} \frac{1}{12} - X_{2\alpha} \cos \theta_p \frac{\pi}{8} \right)
$$

(68)

so the relative energy fluctuation is

$$
\sqrt{\left\langle \delta \hat{H}^2 \right\rangle_\alpha_\alpha} = \frac{\sqrt{\lambda_\alpha(\theta_p)}}{\left| (X_{1\alpha} \frac{1}{12} - X_{2\alpha} \cos \theta_p \frac{\pi}{8}) \right|}
$$

(69)

This expression only applies to the $\lambda_1(\theta_p)$, $\lambda_2(\theta_p)$ eigenvalues, since for $\lambda_3(\theta_p)$ we have $\left\langle \hat{H} \right\rangle_3 = 0$. 

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