SPIN SQUEEZING AND
OTHER ENTANGLEMENT TESTS FOR
TWO MODE SYSTEMS OF
IDENTICAL BOSONS

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Abstract
The concept of entangled quantum states is considered in the context of systems of identical particles, based on the requirement that in order to represent physical states both for the overall system and the sub-systems which may be entangled, the density operators must satisfy the symmetrisation principle and global and local super-selection rules that prohibit states in which there are coherences between differing particle numbers. These requirements and their justification are fully discussed. In the second quantisation approach used, both the system and the sub-systems are modes (or sets of modes) rather than particles, particles being associated with different occupancies of the modes. The definition of entangled states is based on first defining the non-entangled states - after specifying which modes constitute the sub-systems. This paper mainly focuses on two mode entanglement for massive bosons. Several inequalities involving variances and mean values of operators involving mode annihilation, creation operators have been proposed as tests for two mode entangled states, including the inequalities that define spin squeezing. Spin squeezing criteria in two mode systems are examined, and spin squeezing is best considered for principle spin operator components where the covariance matrix is diagonal. It is shown that the presence of spin squeezing in at least one of the spin components requires entanglement of the relevant pair of modes. Several of the other proposed tests for entanglement, including ones based on the sum of the variances for two spin components are considered. All of the tests are still valid when the present concept of entanglement based on the symmetrisation and super-selection rule criteria is applied, but further tests have been obtained here. Sometimes the new tests are satisfied whilst than those obtained in other papers are not.

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1 Introduction

Since the EPR paradox of Einstein et al. [1] on the conflict between quantum theory and local realism, the famous cat paradox of Schrödinger [2] in which the cat could be thought of as being simultaneously dead and alive, and the derivation by Bell et al. [3], [4] of inequalities based on treating measured quantities via a classical hidden variable theory which certain quantum quantum systems violated, entanglement has been recognised as being one of the key features that distinguishes quantum physics from classical physics. It is a feature that arises in the context of composite quantum systems composed of distinct components or sub-systems and is distinct from other features of quantum physics such as quantization for measurements of physical quantities, probabilistic outcomes for such measurements, uncertainty principles involving pairs of physical quantities and so on. Such sub-systems are usually associated with sub-sets of the physical quantities applying to the overall system, and in general more than one choice of sub-systems can be made. The formalism of quantum theory treats pure states for systems made up of two or more distinct sub-systems via tensor products of sub-system states, and since these product states exist in a Hilbert space, it follows that linear combinations of such products could also represent possible pure quantum states for the system. Such quantum superpositions which cannot be expressed as a single product of sub-system states are known as entangled (or non-separable) states. The concept of entanglement can also be extended to mixed states, where quantum states for the system and the sub-systems are specified by density operators. The detailed definition of entangled states is set out in Section 2. This definition is based on first carefully defining the non-entangled (or separable) states such that all non-entangled states must be possible physical states, and in addition these states must be preparable via processes involving separate operations on each sub-system after which correlated sub-system quantum states are combined in accordance with classical probabilities. Thus, although the sub-system states retain their quantum natures the combination resulting in the overall system state is formed classically rather than quantum mechanically. This overall process then involves local operations on the distinct sub-systems and classical communication (LOCC) to prepare a general non-entangled state. The entangled states are then just the physical states which are not non-entangled states. The general idea that in all composite systems the non-entangled states all involve LOCC preparation processes was first suggested by Werner [5]. The notion of physical states, the nature of the systems and sub-systems involved and the specific features required in the definition of non-entangled states when identical particles are involved is discussed in detail in Section 2. Entangled states underlie a number of effects that cannot be interpreted in terms of classical physics, including spin squeezing, non-local measurement correlations - such as for the Einstein-Podolski-Rosen (EPR) paradox and violations of Bell Inequalities. More recently, entangled
states have been recognised as a resource that can be used in various quantum technologies for applications such as teleportation, quantum cryptography, quantum computing and so on. Recent expositions on the effects of entanglement and its role in quantum information science include [6], [7], [8], [9], [10], [11].

It would be pointless to characterise states as entangled unless such states have some important properties. The key requirement is that entangled states exhibit a novel quantum feature that is only found in composite systems. As will be seen in SubSection 2.3 separable states are such that the joint probability for measurements of all physical quantities associated with the sub-systems can be found from separate measurement probabilities obtained from the sub-system density operators and the overall classical probability for creating particular products of sub-system states. Entangled states do not exhibit this feature of separable probabilities, and it is this key non-separability feature that led Schrodinger to call these states "entangled". Hidden variable theories (HVT) (see SubSection 2.5) applied to quantum systems - which are essentially classical in nature - also have the same separability feature for joint probabilities as quantum separable states, though of course the basic concepts are different. The fact that only entangled states do not exhibit the feature of separable probabilities shown in classical HVT highlights entanglement being a non-classical feature found only in composite systems.

It is now generally recognised that entanglement is a relative concept ([12], [13], [14]), [8], [15], [16] and not only depends on the quantum state under discussion but also on which sub-systems are being considered as entangled (or non-entangled). A quantum state may be entangled for one choice of the sub-systems but may be non-entangled if another choice of sub-systems is made, an example being for the hydrogen atom [14] where energy eigenstates are non-entangled if the sub-systems refer to the centre of mass and the relative position of the electron from the proton, but which would be entangled if the sub-systems were the positions of the electron and proton. An example involving two different choices of single particle states in a two mode Bose condensate is given in Section 4.

For a general quantum state various measures of entanglement have been defined - see [8], [9], [15], [16], [17], [18], [19], for details of these, and are aimed at quantifying entanglement to determine which states are more entangled than others. This is important since entanglement is considered as a resource needed in various quantum technologies. Calculations based on such measures of entanglement confirm that for some choices of sub-systems the quantum state is entangled, for others it is non-entangled. For two mode pure states the entanglement entropy - being the difference between the entropy for the pure state (zero) and that associated with the reduced density operator for either of the two sub-systems - is a useful entanglement measure. As entropy and information changes are directly linked [8], [9], this measure is of importance to quantum information science. Another entanglement measure is particle entanglement entropy, defined by Wiseman et al [20], [21], [17] for identical particle systems and based on projecting the quantum state onto states with definite particle
numbers.

Although not directly relatable to the various quantitative measures of entanglement, the results for certain measurements can play the role of being signatures or witnesses or tests of entanglement \[15, 16, 17\]. These are in the form of inequalities for variances and mean values for certain physical quantities, which are consequent on the inequalities that would apply for non-entangled quantum states. If such inequalities are violated then it can be concluded that the state is entangled for the relevant sub-systems. It cannot be emphasised enough that these tests provide sufficiency conditions for establishing that a state is entangled. The failure of a test does not guarantee non-entanglement - sufficiency does not imply necessity. The violation of a Bell inequality is an example of such a signature of entanglement, and the demonstration of spin squeezing is regarded as another. However, the absence of spin squeezing (for example) does not guarantee non-entanglement, as the case of the NOON state in SubSection \[4.3\] shows. A significant number of such inequalities have now been proposed and such signatures of entanglement are the primary focus of the present paper, which is aimed at identifying which of these inequalities really do identify entangled states, especially in the context of two mode systems of identical bosons.

At present there is no clear linkage between quantitative measures of entanglement (such as entanglement entropy) and the quantities used in conjunction with the various entanglement tests (such as the relative spin fluctuation in spin squeezing experiments). Results for experiments demonstrating such non-classical effects cannot yet be used to say much more than the state is entangled, whereas ideally these experiments should determine how entangled the state is. Again we emphasise that neither the entanglement tests nor the entanglement measures are being used to define entanglement. Entanglement is defined first as being the quantum states that are non-separable, the tests for and measures of entanglement are consequential on this definition.

This paper deals with identical particles - bosons or fermions. In the second quantisation approach used here the system is regarded as a set of quantum fields, each of which may be considered as a collection of single particle states or modes. Hence both the system and sub-systems will be specified via the modes that are involved, so here the sub-systems in terms of which non-entangled (and hence entangled) states are defined are modes or sets of modes, not particles \[12, 13, 14\], \[8, 22, 23\]. In this approach, particles will be described via the occupancies of the various modes, so that situations with differing numbers of particles will be treated as differing quantum states of the same system, not as different systems - as in the first quantisation approach. Note that the choice of modes is not unique - original sets of orthogonal one particle states (modes) may be replaced by other orthogonal sets. An example is given in Section \[3\].

Modes can often be categorised as localised modes, where the corresponding single particle wavefunction is confined to a restricted spatial region, or may be categorised as delocalised modes, where the opposite applies. Single particle harmonic oscillator states are an example of localised modes, momentum states are an example of delocalised modes. This distinction is significant when
phenomena such as EPR violations and teleportation are considered.

Although multi-mode systems are also considered, in this paper we mainly focus on two mode systems of identical bosonic atoms, where the atoms at most occupy only two single particle states or modes. For bosonic atoms this situation applies in two mode interferometry, where if a single hyperfine component is involved the modes concerned may be two distinct spatial modes, such as in a double well magnetic or optical trap, or if two hyperfine components are involved in a single well trap each component has its own spatial mode. Large numbers of bosons may be involved since there is no restriction on the number of bosons that can occupy a bosonic mode. For fermionic atoms each hyperfine component again has its own spatial mode. However, if large numbers of fermionic atoms are involved then as the Pauli exclusion principle only allows each mode to accommodate one fermion, it follows that a large number of modes must considered and two mode systems would be restricted to at most two fermions. Consideration of multi-mode entanglement for large numbers of fermions is outside the scope of the present paper (see [24] for a treatment of this), and unless otherwise indicated the focus will be on bosonic modes. The paper focuses on identical bosonic atoms - whether the paper also applies to photons is less clear and will be discussed below.

The work presented here begins with the fundamental issue of how an entangled state should be defined in the context of systems involving identical particles. To reiterate - in the commonly used mathematical approach for defining entangled states, this requires first defining a general non-entangled state, all other states therefore being entangled. We adhere to the original definition of Werner [5] in which the separable states are those that can be prepared by LOCC. This approach is adopted by other authors, see for example [25], [26], [27]. However, in other papers - see for example [28], [29] so-called separable non-local states are introduced in which LOCC is not required (see SubSection 2.13 for an example). It is contended here that the density operators both for the overall system states and for the sub-system states of non-entangled states must represent physical states and in some other work (discussed below) this is not the case. A key feature required of all physical states for systems involving identical particles, entangled or not is that they satisfy the symmetrization principle. This places restrictions both on the form of the overall density operator and also on what can be validly considered to be a sub-system. In particular this rules out individual identical particles being treated as sub-systems, as is done in some papers (see below). In addition, super-selection rules (SSR) only allow density operators which have zero coherences between states with differing total numbers of particles to represent valid physical states, and this will be taken into account for all physical states of the overall system, entangled or not. This is referred to as the global particle number super-selection rule. In non-entangled or separable states the density operator is a sum over products of sub-system density operators, each product being weighted by its probability of occurring (see below for details). For the non-entangled or separable states, a so-called local particle number super-selection rule will also be applied to the density operators describing each of the sub-systems. These sub-system density opera-
tors must then have zero coherences between states with differing numbers of *sub-system particles*. This additional restriction excludes density operators as defining non-entangled states when the sub-system density operators do not conform to the local particle number super-selection rule. Consequently, density operators where the local particle number SSR does not apply would be regarded as entangled states. This viewpoint is discussed in papers by Bartlett et al [25], [31] as one of several approaches for defining entangled states. However, other authors such as [28], [29] state on the contrary that states when the sub-system density operators do *not* conform to the local particle number super-selection rule are still separable, others such as [32], [33] do so by implication. So in this paper we are advocating a *different definition* to some *other definitions* of entanglement in identical particle systems, the consequence being that the set of entangled states is now much *larger*. This is a *key idea* in this paper - not only should super-selection rules on particle numbers be applied to the *overall* physical state, entangled or not, but it *also* should be applied to the density operators that describe states of the modal *sub-systems* involved in the general definition of *non-entangled* states.

The detailed reasons for adopting this viewpoint are set out below. As will be seen, the local particle number super-selection rule restriction *firstly* depends on the *fundamental requirement* that for *all* composite systems - whether identical particles are involved or not - non-entangled states are only those that can be prepared via processes that involve only local operations and classical communication (LOCC). The requirement that the sub-system density operators in identical particle cases satisfy the local particle number SSR is *consequential* on the sub-system states being possible physical sub-system states. As mentioned before, the general definition of non-entangled states based on LOCC preparation processes was first suggested by Werner [5]. Apart from the papers by Bartlett et al [25], [31] we are not aware that this LOCC/SSR based criteria for non-entangled states has been invoked previously for identical particle systems, indeed the opposite approach has been proposed [28], [29]. However, the idea of considering whether sub-system states should satisfy the local particle number SSR has been presented in several papers - [28], [29], [25], [31], [34], [35], [36], mainly in the context of pure states for bosonic systems, though in these papers the focus is on issues other than the definition of entanglement - such as quantum communication protocols [25], multicopy distillation [25], mechanical work and accessible entanglement [34], [35] and Bell inequality violation [36]. The consequences for entanglement of applying this super-selection rule requirement to the sub-system density operators are quite *significant*, and in the present paper important *new entanglement tests* are determined. Not only can it immediately be established that spin squeezing *requires* entangled states, but though several of the other inequalities (see below) that have been used as signatures of entanglement are still valid, *additional tests* can be obtained which only apply to entangled states that are defined to conform to the symmetrisation principle and the super-selection rules.

It is worth emphasising that requiring the sub-system density operators satisfy the local particle number SSR means that there are less states than other-
wise would be the case which are classed as non-entangled, and *more states* will be regarded as *entangled*. It is therefore not surprising that additional tests for entanglement will result. If *further restrictions* are placed on the sub-system density operator - such as requiring them to correspond to a fixed number of bosons again there will be more states regarded as entangled, and even more entanglement tests will apply. A particular example is given in SubSection 5.3 where the sub-systems are restricted to one boson states.

The *symmetrisation* requirement for systems involving identical particles is well established since the work of Dirac. There are two types of justification for applying the *super-selection rules* for systems of identical particles. The first approach is based on simple considerations and will be outlined here. The second approach is more sophisticated and involves linking the absence or presence of SSR to whether or not there is a suitable *reference frame* in terms of which the quantum state is described [37], [38], [39], [28], [29], [40], [41], [42], [31], [34], [35], [17]. This approach will be described in SubSection 2.10 and Appendix 12.

The key idea being that SSR are a consequence of considering the description of a quantum state by an external observer (Charlie) whose phase reference frame has an *unknown phase difference* from that of an observer ((Alice) more closely linked to the system being studied. Thus, whilst Alice’s description of the quantum state may violate the SSR, the description of the *same* quantum state by Charlie will not. In the main part of this paper the density operator $\hat{\rho}$ used to describe the various quantum states will be that of the external observer (Charlie). Note that if the relationship between the phase references is *known*, then the SSR can be challenged (see SubSection 2.11 and Appendix 12).

Returning to the more simple reasons referred to for invoking the superselection rule to exclude quantum superposition states with differing numbers of identical particles (both massive and otherwise), these may be summarised as:

1. No way is known for creating such states.
2. No way is known for measuring all the properties of such states, even if they existed.
3. Coherence and interference effects can be understood without invoking the existence of such states.
4. The stability of such states against decoherence processes may not be great, so even if they could be created, they could rapidly change to other states. However, decoherence time scales that are not too short would be acceptable, so this last reason is of lesser importance.

Invoking the physical existence of states that as far as we know cannot be made or measured, and for which there are no known physical effects that require their presence seems a rather unnecessary feature to add to the non-relativistic quantum physics of many body systems or to quantum optics, and considerations based on the general principle of simplicity (Occam’s razor) would suggest not doing so until a clear physical justification for including them is found. Furthermore, experiments can be carried out on each of the mode sub-systems considered as a *separate system*, and essentially the *same reasons* that justify applying the super-selection rule to the overall system also apply to the separate mode sub-systems in the context of defining *non-entangled states*. 
Hence, unless it can be justified to ignore the super-selection rule for the overall system it would be *inconsistent* not to apply it to the sub-system as well. The *onus* is on those who wish to ignore the super-selection rule for the separate modes to justify why it is being applied to the overall system. In addition, *joint measurements* on all the sub-systems can be carried out, and the interpretation of the measurement probabilities requires the density operators for the sub-system states to be physically based. The general application of super-selection rules has however been challenged (see SubSection 2.10) on the basis that super-selection rules are not a fundamental requirement of quantum theory, but are restrictions that could be lifted if there is a suitable system that acts as a *reference* for the coherences involved. In Section 2 and related Appendix 13 an analysis of these objections to the super-selection rule is presented, and in Appendix 12 we see that the approach based on phase reference frames does indeed justify the application of the SSR both to the general quantum states for multi-mode systems of identical particles and to the sub-system states for non-entangled states of these systems.

The other focus of this paper is on *spin squeezing*. Heisenberg Uncertainty Principle inequalities involving spin operators [43] and the consequent property of spin squeezing have been well-known in quantum optics for many years. The importance of spin squeezing in quantum metrology is discussed in the paper by Kitagawa et al [44] for general spin systems. It was suggested in this paper that correlations between the individual spins was needed to produce spin squeezing, though no quantitative proof was presented and the more precise concept of entanglement was not mentioned. For the case of two mode systems the earliest paper linking spin squeezing to entanglement is that of Sorensen et al [45], which considers a system of identical bosonic atoms, each of which can occupy one of two internal states. This paper states that spin squeezing requires the quantum state to be entangled, with a proof given in the Appendix. A consideration of how such spin squeezing may be generated via collisional interactions is also presented. The paper by Sorensen et al is often referred to as establishing the link between spin squeezing and entanglement - see for example Michel et al [46], Toth et al [47], Hyllus et al [48]. However, the paper by Sorensen et al [45] is based on a definition of non-entangled states in which the sub-systems are the identical particles, and this is inconsistent with the symmetrization principle. The present paper establishes the link between spin squeezing and entanglement based on a definition of entanglement consistent with the system and sub-system density operators representing physical states.

It is also important to consider which *components* of the spin operator vector are squeezed, and this issue is also considered in the present paper. In the context of the present second quantisation approach to identical particle systems the three spin operator components for two mode systems are expressed in terms of the annihilation, creation operators for the two chosen modes. Spin squeezing can be defined (see Section 3) in terms of the variances of these spin operators, however the *covariance matrix* for the three spin operators will in general have off-diagonal elements, and spin squeezing is better defined in terms of rotated spin operators referred to as *principal spin operators* for which...

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the covariance matrix is \textit{diagonal}. The principal spin operators are related to new mode annihilation, creation operators in the same form as for the original spin operators, where the \textit{new modes} are two orthogonal linear combinations of the originally chosen modes. In discussing the relationship between spin squeezing and entanglement, the modes which may be entangled are generally those associated with the definition of the spin operators.

The plan of this paper is as follows. In Section 2 the key definitions of entangled states are covered, along with detailed discussion on why the symmetrisation principle and the super-selection rule is invoked. Challenges to the necessity of the super-selection rule are outlined, with arguments against such challenges dealt with in Appendices 12, 13, and 14. The next Section 3 sets out the definitions of spin squeezing and in the following Section 4 it is shown that spin squeezing is a signature of entanglement, both for the principle spin operators with entanglement of the two new modes and for the original spin operators with entanglement of the original modes. A number of other tests for entanglement proposed by other authors are considered in Section 5, with details of these treatments set out in Appendices 15, 16, 17. Two key mathematical inequalities are derived in Appendix 10. The final Section 7 summarises and discusses the key results.
2 Entanglement

2.1 Physical States

The standard quantum theory notions of physical systems that can exist in various states and have associated quantities on which measurements can be made are presumed in this paper. The measuring system made be also treated via quantum theory, but there is always some component that behaves classically, so that quantum fluctuations in the quantity recorded by the observer are small.

The term physical state refers to a state that can either be prepared via a process consistent with the laws of quantum physics and on which measurements can be then performed and the probabilistic results predicted from this state (prediction), or a state whose existence can be inferred from later quantum measurements (retrodiction). In quantum theory, physical states are represented by density operators for mixed states or state vectors for pure states, which must satisfy symmetrisation and other basis requirements in accordance with the laws of quantum theory. The quantum state, the system it is associated with and the quantities that can be measured are viewed here as entities that are viewed as being both ontological and epistimological. The observer is important, but there is actually something out there to be studied. In addition to those associated with physical states, other density operators and state vectors may be introduced for mathematical convenience. For physical states, the density operator is determined from either the preparation process or inferred from the measurement process, and in general it is a statistical mixture of density operators for possible preparation processes. Measurement itself constitutes a possible preparation process. Following preparation, further experimental processes may change the physical state and dynamical equations give the time evolution of the density operator between preparation and measurement, the simplest situation being where measurement takes place immediately after preparation. A full discussion of the predictive and retrodictive aspects of the density operator is given in papers by Pegg et al [49], [50]. Whilst there are often different mathematical forms for the density operator that lead to the same predictive results for subsequent measurements, applying the results of the measurements to retrodictively determines the preferred form of the density operator that is consistent with the available preparation and measurement operators. An example is given in [50].

2.2 Entangled and Non-Entangled States

2.2.1 General Considerations

Here the commonly applied mathematical approach to defining entangled states will be described [9]. The definition involves vectors and density operators that represent states that can be prepared in real experiments, so the mathematical approach is to be physically based. The formal definition of what is meant by an entangled state starts with the pure states, described via a vector in a Hilbert space. The formalism of quantum theory treats pure states for composite
systems made up of two or more distinct sub-systems via tensor products of sub-system states

\[ |\Phi \rangle = |\Phi_A \rangle \otimes |\Phi_B \rangle \otimes |\Phi_C \rangle \ldots \]  

Such products are called non-entangled or separable states. However, since these product states exist in a Hilbert space, it follows that linear combinations of such products of the form \( |\Phi \rangle = \sum_{\alpha,\beta} C_{\alpha\beta} |\Phi_A^\alpha \rangle \otimes |\Phi_B^\beta \rangle \otimes |\Phi_C^{..} \rangle \ldots \) could also represent possible pure quantum states for the system. Such quantum superpositions which cannot be expressed as a single product of sub-system states are known as entangled (or non-separable) states.

The concept of entanglement can be extended to mixed states, which are described via density operators in the Hilbert space. If \( A, B, \ldots \) are the sub-systems with \( \hat{\rho}_R^A, \hat{\rho}_R^B, \ldots \) being density operators the sub-systems \( A, B, \ldots \), then a general non-entangled or separable state is one where the overall density operator \( \hat{\rho} \) can be written as the weighted sum of tensor products of these sub-system density operators in the form

\[ \hat{\rho} = \sum_R P_R \hat{\rho}_R^A \otimes \hat{\rho}_R^B \otimes \hat{\rho}_R^C \otimes \ldots \]  

with \( \sum_R P_R = 1 \) and \( P_R \geq 0 \) giving the probability that the specific product state \( \hat{\rho}_R = \hat{\rho}_R^A \otimes \hat{\rho}_R^B \otimes \hat{\rho}_R^C \otimes \ldots \) occurs. Entangled states (or non-separable states) are those that cannot be written in this form, so in this approach knowing what the term entangled state refers to is based on first knowing what the general form is for a non-entangled state.

The key requirement is that entangled states exhibit a novel quantum feature that is only found in composite systems. Separable states are such that the joint probability for measurements of all physical quantities associated with the sub-systems can be found from separate measurement probabilities obtained from the sub-system density operators \( \hat{\rho}_R^A, \hat{\rho}_R^B, \ldots \) and the overall classical probability \( P_R \) (see SubSection 2.3). This feature of separable probabilities is absent in entangled states, and because of this key non-separability feature Schrödinger called these states “entangled”. The separability feature for the joint probabilities is essentially a classical feature and applies in hidden variable theories.
(HVT) (see SubSection 2.5) applied to quantum systems - as well as to quantum separable states. The fact that only entangled states do not exhibit the feature of separable probabilities shown in classical HVT highlights entanglement being a non-classical feature found only in composite systems.

An alternative operational approach to defining entangled states focuses on whether or not they exhibit certain non-classical features such as Bell Inequality violation or whether they satisfy certain mathematical tests such as having a non-negative partial transpose \[^{[51]}^{[15]}\] and a utilitarian approach focuses or whether entangled states have technological applications such as in various quantum information protocols. As will be seen in SubSection 2.12 the particular definition of entangled states based on their non-creatability via LOCC essentially coincides with the approach used in the present paper. Wiseman et al. \[^{[52]}^{[26]}\] and Reid et al. \[^{[11]}\] discuss the concept of a hierarchy of entangled states, with states exhibiting Bell nonlocality being a subset of states for which there is EPR steering, which in turn is a subset of the entangled states, the latter being defined as states whose density operators cannot be written as in Eq. \(^2\) though without further consideration if additional properties are required for the sub-system density operators. The operational approach could lead into a quagmire of differing interpretations of entanglement depending on which non-classical feature is highlighted, and the utilitarian approach implies that all entangled states have a technological use, which is by no means the case. For these reasons, the present mathematical approach based on the quantities involved representing physical sub-system states is generally favoured \[^{[9]}\]. It is also compatible with later classifying entangled states in a hierarchy.

### 2.2.2 Local Systems and Operations

As pointed out by Vedral \[^{[8]}\], one reason for calling states such as in Eqs. \(^1\) and \(^2\) separable is associated with the idea of performing operations on the separate sub-systems that do not affect the other sub-systems. Such operations on such local systems are referred to as local operations and include unitary operations \(\hat{U}_A, \hat{U}_B\), that change the states via \(\hat{\rho}_R^A \rightarrow \hat{U}_A^* \hat{\rho}_R^A \hat{U}_A, \hat{\rho}_R^B \rightarrow \hat{U}_B \hat{\rho}_R^B \hat{U}_B^*\), etc as in a time evolution, and could include processes by which the states \(\hat{\rho}_R^A, \hat{\rho}_R^B\), are separately prepared from suitable initial states.

We note that performing local operations on a separable state only produces another separable state, not an entangled state. Such local operations are obviously facilitated in experiments if the sub-systems are essentially non-interacting - such as when they are spatially well-separated, though this does not have to be the case. The local systems and operations could involve sub-systems whose quantum states and operators are just in different parts of Hilbert space, such as for cold atoms in different hyperfine states even when located in the same spatial region. Note the distinction between local and localised. As described by Werner \[^{[5]}\], if one observer (Alice) is associated with preparing separate sub-system \(A\) in a physical state \(\hat{\rho}_R^A\) via local operations with a probability \(P_R\), a second observer (Bob) could be then advised via a classical communication channel to prepare sub-system \(B\) in state \(\hat{\rho}_R^B\) via local operations. After repeating this process
for different choices $R$ of the correlated pairs of sub-system states, the overall quantum state prepared by both observers via this local operation and classical communication protocol (LOCC) would then be the bipartite non-entangled state $\hat{\rho} = \sum_R P_R \hat{\rho}_R^A \otimes \hat{\rho}_R^B$. Multiparticle non-entangled states of the form (2) can also be prepared via LOCC protocols involving further observers. As will be seen, the separable or non-entangled states are just those that can be prepared by LOCC protocols.

2.2.3 Constraints on Sub-System Density Operators

A key issue however is whether density operators $\hat{\rho} \; \hat{\rho}_R^A \; \hat{\rho}_R^B$, in Eq. (2) always represent possible physical states, even if the operators $\hat{\rho}, \hat{\rho}_R^A, \hat{\rho}_R^B$, etc satisfy all the standard mathematical requirements for density operators - Hermitian, positiveness, trace equal to unity, trace of density operator squared being not greater than unity. In this paper it will be argued that there are further requirements not only on the overall density operator, but also on those for the individual sub-systems that are imposed by symmetrisation and super-selection rules.

2.3 Separate and Joint Measurements, Reduced Density Operator

In this SubSection we consider separate and joint measurements on systems involving several sub-systems and introduce results for probabilities, mean values for measurements on one of the sub-systems which are conditional on the results for measurements on another of the sub-systems. This will require consideration of quantum theoretical conditional probabilities. The measurements involved will be assumed for simplicity to be von Neumann projective measurements for physical quantities represented by Hermitian operators $\hat{\Omega}$, which project the quantum state into subspaces for the eigenvalue $\lambda_i$ that is measured, the subspaces being associated with Hermitian, idempotent projectors $\hat{\Pi}_i$, whose sum over all eigenvalues is unity. These concepts are treated in several quantum theory textbooks, for example [6], [53]. For completeness, an account setting out the key results is presented in Appendix 9.

2.3.1 Joint Measurements on Sub-Systems

For situations involving distinct sub-systems measurements can be carried out on all the sub-systems and the results expressed in terms of the joint probability for various outcomes. If $\hat{\Omega}_A$ is a physical quantity associated with sub-system $A$, with eigenvalues $\lambda_i^A$ and with $\hat{\Pi}_i^A$ the projector onto the subspace with eigenvalue $\lambda_i^A$, $\hat{\Omega}_B$ is a physical quantity associated with sub-system $B$, with eigenvalues $\lambda_j^B$ and with $\hat{\Pi}_j^B$ the projector onto the subspace with eigenvalue $\lambda_j^B$ etc., then the joint probability $P_{AB..(i,j,..)}$ that measurement of $\hat{\Omega}_A$ leads
to result $\lambda^A_i$, measurement of $\hat{\Omega}_B$ leads to result $\lambda^B_j$, etc is given by

$$P_{AB..}(i, j, ..) = Tr(\hat{\Pi}^A_i \hat{\Pi}^B_j .. \hat{\rho})$$ (3)

This joint probability depends on the full density operator $\hat{\rho}$ representing the physical state as well as on the quantities being measured. Here the projectors (strictly $\hat{\Pi}^A_i \otimes \hat{\Pi}^B_j ..$, $\hat{\Pi}^A_i \otimes \hat{\Pi}^B_j ..$, etc) commute, so the order of measurements is immaterial. An alternative notation in which the physical quantities are also specified is $P_{AB..}(\hat{\Omega}_A, i; \hat{\Omega}_B, j; ..)$.

### 2.3.2 Single Measurements on Sub-Systems and Reduced Density Operator

The reduced density operator $\hat{\rho}_A$ for sub-system $A$ given by

$$\hat{\rho}_A = Tr_{B,C,..}(\hat{\rho})$$ (4)

and enables the results for measurements on sub-system $A$ to be determined for the situation where the results for all joint measurements involving the other sub-systems are discarded. The probability $P_A(i)$ that measurement of $\hat{\Omega}_A$ leads to result $\lambda^A_i$ irrespective of the results for measurements on the other sub-systems is given by

$$P_A(i) = \sum_{j,k,..} P_{AB..}(i, j, ..)$$

$$= Tr(\hat{\Pi}^A_i \hat{\rho})$$ (5)

$$= Tr_A(\hat{\Pi}^A_i \hat{\rho}_A)$$ (6)

using $\sum_j \hat{\Pi}^B_j = \hat{1}$, etc. Hence the reduced density operator $\hat{\rho}_A$ plays the role of specifying the physical state for mode $A$ considered as a separate sub-system, even if the original state $\hat{\rho}$ is entangled. An alternative notation in which the physical quantity is also specified is $P_A(\hat{\Omega}_A, i)$.

### 2.3.3 Mean Value and Variance

The mean value for measuring a physical quantity $\hat{\Omega}_A$ will be given by

$$\langle \hat{\Omega}_A \rangle = \sum_{\lambda^A_i} \lambda^A_i P_A(i)$$

$$= Tr_A(\hat{\Omega}_A^A \hat{\rho}_A)$$ (7)

where we have used $\hat{\Omega}_A = \sum_{\lambda^A_i} \lambda^A_i \hat{\Pi}^A_i$.

The variance of measurements of the physical quantity $\hat{\Omega}_A$ will be given by

$$\langle (\Delta \hat{\Omega}_A)^2 \rangle = \sum_{\lambda^A_i} (\lambda^A_i - \langle \hat{\Omega}_A \rangle)^2 P_A(i)$$

$$= Tr_A((\hat{\Omega}_A^A - \langle \hat{\Omega}_A \rangle^2 \hat{\rho}_A)$$ (8)
so both the mean and variance only depend on the reduced density operator $\hat{\rho}_A$.

On the other hand the *mean value* of a product of sub-system operators $\hat{\Omega}_A \otimes \hat{\Omega}_B \otimes \hat{\Omega}_C \otimes ...$, where $\hat{\Omega}_A, \hat{\Omega}_B, \hat{\Omega}_C, ..$ are Hermitian operators representing physical quantities for the separate sub-systems, is given by

$$\left\langle \hat{\Omega}_A \otimes \hat{\Omega}_B \otimes \hat{\Omega}_C \otimes ... \right\rangle = \sum_{\lambda^A} \sum_{\lambda^B} ... \lambda^A_i \lambda^B_j ... P_{AB..}(i,j,..)$$

which involves the overall system density operator, as expected.

### 2.3.4 Conditional Probabilities

Treating the case of two sub-systems for simplicity we can use Bayes theorem (see Appendix 9, Eq.(252)) to obtain expressions for conditional probabilities [9]. The conditional probability that if measurement of $\hat{\Omega}_B$ associated with sub-system $B$ leads to eigenvalue $\lambda^B_j$ then measurement of $\hat{\Omega}_A$ associated with sub-system $A$ leads to eigenvalue $\lambda^A_i$ is given by

$$P_{AB}(i|j) = Tr(\hat{\Pi}_A^i \hat{\Pi}_B^j \hat{\rho}) / Tr(\hat{\Pi}_B^j \hat{\rho})$$

In general, the overall density operator is required to determine the conditional probability. An alternative notation in which the physical quantities are also specified is $P_{AB}(\hat{\Omega}_A, i | \hat{\Omega}_B, j)$.

As shown in Appendix 9 the conditional probability is given by

$$P_{AB}(i|j) = Tr(\hat{\Pi}_A^i \hat{\rho}_{\text{cond}}(\hat{\Omega}_B, \lambda^B_j))$$

where

$$\hat{\rho}_{\text{cond}}(\hat{\Omega}_B, \lambda^B_j) = \hat{\Pi}_B^j \hat{\rho} \hat{\Pi}_B^j / Tr(\hat{\Pi}_B^j \hat{\rho})$$

is the so-called *conditioned density operator*, corresponding the quantum state produced following the measurement of $\hat{\Omega}_B$ that obtained the result $\lambda^B_j$. The conditional probability result is the same as

$$P_{AB}(i|j) = Tr(\hat{\Pi}_A^i \hat{\rho}_{\text{cond}}(\hat{\Omega}_B, \lambda^B_j))$$

which is the same as the expression [9] with $\hat{\rho}$ replaced by $\hat{\rho}_{\text{cond}}(\hat{\Omega}_B, \lambda^B_j)$. This is what would be expected for a conditioned measurement probability.

Also, if the measurement results for $\hat{\Omega}_B$ are not recorded the conditioned density operator now becomes

$$\hat{\rho}_{\text{cond}}(\hat{\Omega}_B) = \sum_{\lambda^B_j} P_B(j) \hat{\rho}_{\text{cond}}(\hat{\Omega}_B, \lambda^B_j)$$

$$= \sum_{\lambda^B_j} \hat{\Pi}_B^j \hat{\rho} \hat{\Pi}_B^j$$

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This is still different to the original density operator \( \hat{\rho} \) because a measurement of \( \hat{\Omega}_B \) has occurred, even if we don’t know the outcome. However, the measurement probability for \( \hat{\Omega}_A \) is now

\[
P_{AB}(i|\text{Any } j) = Tr(\hat{\Pi}^A_i \hat{\rho}_{\text{cond}}(\hat{\Omega}_B))
\]

\[
= Tr(\hat{\Pi}^A_i \hat{\rho})
\]

\[
= P_A(i)
\]

where we have used the cyclic properties of the trace, \( (\hat{\Pi}_j^B)^2 = \hat{\Pi}_j^B \) and \( \sum_{j} \lambda_j B \hat{\Pi}_j^B = 1 \). The results in Eqs. (15) and (16) are the same as the measurement probability for \( \hat{\Omega}_A \) if no measurement for \( \hat{\Omega}_B \) had taken place at all. This is perhaps not surprising, since the record of the latter measurements was discarded. Another way of showing this result is that Bayes Theorem tells us

\[
\sum_j P_{AB}(i|j) P_B(j) = \sum_j P_{AB}(i,j) = P_A(i),
\]

since \( \sum_j P_{AB}(i,j) \) is the probability that measurement of \( \hat{\Omega}_A \) will lead to \( \lambda_i^A \) and measurement of \( \hat{\Omega}_B \) will lead to any of the \( \lambda_j^B \). This result is called the no-signalling theorem [9].

### 2.3.5 Conditional Mean and Variance

As explained in Appendix 9, to determine the conditioned mean value of \( \hat{\Lambda} \) after measurement of \( \hat{\Omega} \) has led to the eigenvalue \( \lambda_i \) we use \( \hat{\rho}_{\text{cond}}(\hat{\Omega}, i) \) rather than \( \hat{\rho} \) in the mean formula \( \langle \hat{\Lambda} \rangle = Tr(\hat{\Lambda} \hat{\rho}) \) and the result is given in terms of the conditional probability \( P(\hat{\Lambda}, j|\hat{\Omega}) \). Here we refer to two commuting observables and include the operators in the notation to avoid any misinterpretation. Hence

\[
\langle \hat{\Lambda} \rangle_{\hat{\Omega}, i} = Tr(\hat{\Lambda} \hat{\rho}_{\text{cond}}(\hat{\Omega}, i))
\]

\[
= \sum_j \mu_j P(\hat{\Lambda}, j|\hat{\Omega}, i)
\]

For the conditioned variance of \( \hat{\Lambda} \) after measurement of \( \hat{\Omega} \) has led to the eigenvalue \( \lambda_i \) we use \( \hat{\rho}_{\text{cond}}(\hat{\Omega}, i) \) rather than \( \hat{\rho} \) and the conditioned mean \( \langle \hat{\Lambda} \rangle_{\hat{\Omega}, i} \) rather than \( \langle \hat{\Lambda} \rangle \) in the variance formula \( \langle \Delta \hat{\Lambda}^2 \rangle = Tr((\hat{\Lambda} - \langle \hat{\Lambda} \rangle)^2 \hat{\rho}) \). Hence

\[
\langle \Delta \hat{\Lambda}^2 \rangle_{\hat{\Omega}, i} = Tr((\hat{\Lambda} - \langle \hat{\Lambda} \rangle_{\hat{\Omega}, i})^2 \hat{\rho}_{\text{cond}}(\hat{\Omega}, i))
\]

\[
= \sum_j (\mu_j - \langle \hat{\Lambda} \rangle_{\hat{\Omega}, i})^2 P(\hat{\Lambda}, j|\hat{\Omega}, i)
\]

If we weighted the conditioned mean by the probability \( P(\hat{\Omega}, i) \) that measuring \( \hat{\Omega} \) has led to the eigenvalue \( \lambda_i \) and summed over the possible outcomes \( \lambda_i \) for the \( \hat{\Omega} \) measurement, then we obtain the mean for measurements of
\( \hat{\Lambda} \) after un-recorded measurements of \( \hat{\Omega} \) have occurred. From Bayes theorem

\[
\sum_i P(\hat{\Lambda}, j | \hat{\Omega}, i) P(\hat{\Omega}, i) = P(\hat{\Lambda}, j)
\]

so this gives the unrecorded mean \( \langle \hat{\Lambda} \rangle_\hat{\Omega} \) as

\[
\langle \hat{\Lambda} \rangle_\hat{\Omega} = \sum_i \langle \hat{\Lambda} \rangle_{\hat{\Omega}, i} P(\hat{\Omega}, i) \\
= \sum_j \mu_j P(\hat{\Lambda}, j) \\
= \langle \hat{\Lambda} \rangle
\]

which is the usual mean value for measurements of \( \hat{\Lambda} \) when no measurements of \( \hat{\Omega} \) have occurred. Note that no such similar result occurs for the unrecorded variance \( \langle \Delta \hat{\Lambda}^2 \rangle_\hat{\Omega} \)

\[
\langle \Delta \hat{\Lambda}^2 \rangle_\hat{\Omega} = \sum_i \langle \Delta \hat{\Lambda}^2 \rangle_{\hat{\Omega}, i} P(\hat{\Omega}, i) \\
\neq \langle \Delta \hat{\Lambda}^2 \rangle
\]
2.4 Non-Entangled States

In this SubSection we will set out the key results for measurements on non-entangled states.

2.4.1 Non-Entangled States - Joint Measurements on Sub-Systems

In the case of the general non-entangled state we find that the joint probability is

\[ P_{AB..}(i,j,..) = \sum_R P^R_A(i)P^R_B(j) .. \]  

(21)

where

\[ P^R_A(i) = \text{Tr}(\hat{\Pi}^A_i \hat{\rho}_R^A) \quad P^R_B(j) = \text{Tr}(\hat{\Pi}^B_j \hat{\rho}_R^B) \]  

(22)

are the probabilities for measurement results for \( \hat{\Omega}_A, \hat{\Omega}_B, .. \) on the separate sub-systems with density operators \( \hat{\rho}_R^A, \hat{\rho}_R^B, \) etc and the overall joint probability is given by the products of the probabilities \( P^R_A(i), P^R_B(j), .. \) for the measurement results \( \lambda^A_i, \lambda^B_j, .. \) for physical quantities \( \hat{\Omega}_A, \hat{\Omega}_B, .. \) if the sub-systems are in the states \( \hat{\rho}_R^A, \hat{\rho}_R^B, \) etc. These products are then weighted by the probability \( P_R \) that the system is prepared in the particular product state \( \hat{\rho}_R^A \otimes \hat{\rho}_R^B \otimes \hat{\rho}_C^R \otimes .. \) to determine the overall joint probability \( P_{AB..}(i,j,..) \). The overall probability is of a classical form. Obviously this joint probability depends on the sub-system density operators \( \hat{\rho}_R^A, \hat{\rho}_R^B, \) etc.

This key result (21) showing that the joint measurement probability for a separable state only depends on separate measurement probabilities for the sub-systems, together with the classical probability for preparing correlated product states of the sub-systems, does not apply for entangled states. Hence the key quantum feature for composite systems of non-separability for joint measurement probabilities applies only to entangled states. As will be shown below, a similar result to (21) also occurs in hidden variable theory - a classical theory - so non-separability for joint measurements resulting from entanglement is a truly non-classical feature of composite systems.

2.4.2 Non-Entangled States - Single Measurements on Sub-Systems

For the general non-entangled state, the reduced density operator for sub-system A is given by

\[ \hat{\rho}_A = \sum_R P_R \hat{\rho}_R^A \]  

(23)

A key feature of a non-entangled state is that the results of a measurement on any one of the sub-systems is independent of the states for the other sub-systems. From Eqs. (6) and (23) the probability \( P_A(i) \) that measurement of \( \hat{\Omega}_A \) leads to result \( \lambda^A_i \) is given by

\[ P_A(i) = \sum_R P_R P^R_A(i) \]  

(24)
where the reduced density operator is given by Eq. (23) for the non-entangled state in Eq. (2). This result only depends on the reduced density operator $\hat{\rho}_A$, which represents a state for sub-system $A$ and which is a statistical mixture of the sub-system states $\hat{\rho}_A^R_i$, with a probability $P_R$ that is the same for all sub-systems. The result for the measurement probability $P_A(i)$ is just the statistical average of the results that would apply if sub-system $A$ were in possible states $\hat{\rho}_A^R$. For all quantum states the final expression for the measurement probability $P_A(i)$ only involves a trace of quantities $\hat{\Pi}_A^i$, $\hat{\rho}_A$ that apply to sub-system $A$, but for a non-entangled state the reduced density operator $\hat{\rho}_A$ is given by an expression (23) that does not involve density operators for the other sub-systems. Thus for a non-entangled state, the probability $P_A(i)$ is independent of the states $\hat{\rho}_B^R$, $\hat{\rho}_C^R$, associated with the other sub-systems. Analogous results apply for measurements on the other sub-systems.

### 2.4.3 Non-Entangled States - Conditional Probability

For a general non-entangled bipartite mixed state the conditional probability is given by

$$P_{AB}(i|j) = \sum_R P_R P_A^R(i) P_B^R(j) / \sum_R P_R P_B^R(j)$$

(25)

which in general depends on $\hat{\Omega}_B$ associated with sub-system $B$ and the eigenvalue $\lambda_B^j$. This may seem surprising for the case where $A$ and $B$ are localised sub-systems which are well separated. It implies that even for separable states a measurement result for sub-system $B$ will affect the result for a totally unrelated measurement on sub-system $A$ which is a long distance away. This is an example of "spooky action at a distance". However, it should be remembered that the general separable state is still a correlated state, so each sub-system density operator $\hat{\rho}_R$ for sub-system $B$ is matched with a corresponding density operator $\hat{\rho}_A^R$ for sub-system $A$. It is therefore not surprising that the measurement results for $A$ are not independent of those for $B$.

However, for a non-entangled pure state where $\hat{\rho} = \hat{\rho}_A^A \otimes \hat{\rho}_B^B$ we find that

$$P_{AB}(i|j) = P_A(i)$$

(26)

where $P_A(i) = \text{Tr}(\hat{\Pi}_A^i \hat{\rho}_A^A)$. For separable pure states the conditional probability is independent of $\hat{\Omega}_B$ associated with sub-system $B$ and the eigenvalue $\lambda_B^j$.

Also of course $\sum_j P_{AB}(i|j) P_B(j) = P_A(i)$ is true for separable states since it applies to general bipartite states. Hence if the measurement results for $\hat{\Omega}_B$ are discarded then the probability distribution for measurements on $\hat{\Omega}_A$ will be determined from the conditioned density operator $\hat{\rho}_\text{cond}(\hat{\Omega}_B)$ and just result in $P_A(i)$ - as in shown in Eq. (16) for any quantum state.

### 2.4.4 Non-Entangled States - Mean Values and Correlations

For non-entangled states as in Eq. (2) the mean value for measuring a physical quantity $\hat{\Omega}_A \otimes \hat{\Omega}_B \otimes \hat{\Omega}_C \otimes ...$, where $\hat{\Omega}_A$, $\hat{\Omega}_B$, $\hat{\Omega}_C$, .. are Hermitian operators
representing physical quantities for the separate sub-systems can be obtained from Eqs. (2) and (9) and is given by

\[ \langle \hat{\Omega}_A \otimes \hat{\Omega}_B \otimes \hat{\Omega}_C \otimes \rangle = \sum_R R P_R \langle \hat{\Omega}_A \rangle_R^A \langle \hat{\Omega}_B \rangle_R^B \langle \hat{\Omega}_C \rangle_R^C \ldots \] (27)

where

\[ \langle \hat{\Omega}_K \rangle_R^K = \text{Tr}(\hat{\Omega}_K \hat{\rho}_R^K), \quad (K = A, B, \ldots) \] (28)

is the mean value for measuring \( \hat{\Omega}_K \) in the \( K \) sub-system when its density operator is \( \hat{\rho}_R^K \). Since the overall mean value is not equal to the product of the separate mean values, the measurements on the sub-systems are said to be correlated. However, for the general non-entangled state as the mean value is just the products of mean values weighted by the probability of preparing the particular product state - which involves a LOCC protocol, as we have seen - the correlation is classical rather than quantum [9]. In the case of a single product state where \( \hat{\rho} = \hat{\rho}_A^A \otimes \hat{\rho}_B^B \otimes \hat{\rho}_C^C \ldots \) we have \( \langle \hat{\Omega}_A \otimes \hat{\Omega}_B \otimes \hat{\Omega}_C \otimes \rangle = \langle \hat{\Omega}_A \rangle^A \langle \hat{\Omega}_B \rangle^B \langle \hat{\Omega}_C \rangle^C \ldots \) which is just the product of mean values for the separate sub-systems, and in this case the measurements on the sub-systems are said to be uncorrelated. For entangled states however the last result for \( \langle \hat{\Omega}_A \otimes \hat{\Omega}_B \otimes \hat{\Omega}_C \otimes \rangle \) does not apply, and the correlation is strictly quantum.

### 2.5 Hidden Variable Theory

In a general local hidden variable theory physical quantities associated with the sub-systems are denoted \( \Omega_A, \Omega_B \) etc, which are real numbers not operators. Their values are assumed to be \( \lambda_i^A \), \( \lambda_j^B \) etc - the same as in quantum theory, since HVT does not challenge the quantization feature. In the realist viewpoint of HVT all the physical quantities have definite values at any time, these values being determined from a set of hidden variables \( \xi \). Measurement is not required for the values for physical quantities to be created, as in quantum theory. However, in a so-called "fuzzy" hidden variable theory [54] (see also Section 7.1 of [8]) the values for \( \Omega_A, \Omega_B \) etc are determined probabilistically from the hidden variables. For particular hidden variables \( \xi \) the probability that \( \Omega_A \) has value \( \lambda_i^A \) will be given by \( P_A(i, \xi) \), for particular hidden variables \( \xi \) the probability that \( \Omega_B \) has value \( \lambda_j^B \) will be given by \( P_B(j, \xi) \), etc and the HVT joint probability will be given by

\[ P_{AB}(i,j, \ldots) = \int d\xi \frac{d\xi}{P(\xi)} P_A(i, \xi)P_B(j, \xi) \ldots \] (29)

Here \( P(\xi) \) is the probability that the hidden variables are in the range \( d\xi \) around \( \xi \), the HV being assumed continuous - which is not a requirement. The probabilities satisfy the usual sum rules for all outcomes giving one, thus \( \sum_i P_A(i, \xi) = 1 \), etc., \( \int d\xi P(\xi) = 1 \).
The formal similarity of the HVT expression for the joint probability and that for the case of quantum separable states given in Eq. (21) is noticeable. Although the conceptual basis of the various factors is quite different, it is always possible to describe any quantum separable state via a HVT. The different \( R \) for the separable state can be regarded as equivalent to hidden variables \( \xi \), with \( P_R \Rightarrow P(\xi) \) and \( \sum_R \Rightarrow \int d\xi \). The HVT classical probabilities \( P_A(i, \xi), P_B(j, \xi) \) would be given by the quantum probabilities

\[
\text{Tr} (\hat{\Pi}_A^i \hat{\rho}_A^R), \quad \text{Tr} (\hat{\Pi}_B^j \hat{\rho}_B^R),
\]

respectively. There is of course no independent fully developed classical HVT that can predict the \( P_A(i, \xi), P_B(j, \xi) \) etc.

However, as we will see both the HVT and the quantum separable state predictions are consistent with Bell Inequalities, and it requires a quantum entangled state to demonstrate violations. Naturally it follows that quantum entangled states cannot be described via a HVT.

2.5.1 HVT- Mean Values and Correlation

The actual values that would be assigned to the physical quantities \( \Omega_A, \Omega_B \) etc will depend on the hidden variables but can be taken as the mean values of the possible values \( \lambda_i^A, \lambda_i^B \) etc. We denote these mean values as \( \langle \Omega_A(\xi_A) \rangle, \langle \Omega_B(\xi_B) \rangle \) etc where

\[
\langle \Omega_K(\xi_K) \rangle = \sum_{\lambda_K} \lambda_K^k P_K(k, \xi_K) \quad (K = A, B,..)
\]

These expressions may be compared to Eq. (28) for the mean values of physical quantities \( \hat{\Omega}_A, \hat{\Omega}_B \) etc in quantum separable states.

We can then obtain an expression for the mean value in HVT of the physical quantity \( \Omega_A \otimes \Omega_B \otimes \Omega_C \otimes \ldots \), where \( \Omega_A, \Omega_B, \) etc. are physical quantities for the separate sub-systems. This is obtained from Eqs. (29) and (30) and is given by

\[
\langle \Omega_A \otimes \Omega_B \otimes \Omega_C \otimes \ldots \rangle_{HVT} = \int d\xi P(\xi) \langle \Omega_A(\xi_A) \rangle \langle \Omega_B(\xi_B) \rangle \langle \Omega_C(\xi_C) \rangle \ldots
\]

This may be compared to Eq. (27) for the mean value of the physical quantity \( \hat{\Omega}_A \otimes \hat{\Omega}_B \otimes \hat{\Omega}_C \otimes \ldots \) in quantum separable states.

2.5.2 HVT- GHZ State

The GHZ state [55] is an entangled state of three sub-systems \( A, B \) and \( C \), each of which is associated with two quantum states \(|+1\rangle \) and \(|-1\rangle \). Each sub-system has three physical quantities, which are Pauli spin operators \( \hat{\sigma}_x, \hat{\sigma}_y \) and \( \hat{\sigma}_z \). The quantum states \(|+1\rangle \) and \(|-1\rangle \) are eigenstates of \( \hat{\sigma}_z \) with eigenvalues +1 and -1 respectively. Note that the eigenvalues of the other two Pauli spin operators are also +1 and -1. The GHZ state is defined by

\[
|\Psi\rangle_{GHZ} = (|+1\rangle_A |+1\rangle_B |+1\rangle_C + |-1\rangle_A |-1\rangle_B |-1\rangle_C) / \sqrt{2}
\]

The GHZ state provides a clear example of an entangled quantum state which cannot be described via hidden variable theory. In a non-fuzzy version of
HVT each of the nine physical quantities \( \sigma^A_x, \sigma^A_y, \sigma^A_z, \sigma^B_x, \sigma^B_y, \sigma^B_z, \sigma^C_x, \sigma^C_y, \sigma^C_z \) will be associated with hidden variables that directly specify the values \(+1\) and \(-1\) that each one of these physical quantities may have. We denote these hidden variables as \( M^K_\alpha \), where \( K = A, B, C \) and \( \alpha = x, y, z \) and we have \( M^K_\alpha = +1 \) or \(-1\). With this direct specification of the physical values Eq.(30) just becomes

\[
\langle \sigma^K_\alpha(M^K) \rangle = M^K_\alpha
\]

and Eq.(31) becomes

\[
\langle \sigma^A_x \sigma^B_y \sigma^C_z \rangle_{\text{HVT}} = M^A_x M^B_y M^C_z
\]

We can then derive a contradiction with quantum theory regarding the HVT description of the GHZ state.

Firstly, using the Pauli spin matrices for the \(|+1\rangle\) and \(|-1\rangle\) basis states

\[
\begin{align*}
[\hat{\sigma}_x] &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\
[\hat{\sigma}_y] &= \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \\
[\hat{\sigma}_z] &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}
\end{align*}
\]

it is straightforward to show that the GHZ state satisfies three eigenvalue equations

\[
\begin{align*}
\hat{\sigma}^A_x \hat{\sigma}^B_y \hat{\sigma}^C_z |\Psi\rangle_{\text{GHZ}} &= (-1) |\Psi\rangle_{\text{GHZ}} \\
\hat{\sigma}^A_y \hat{\sigma}^B_x \hat{\sigma}^C_y |\Psi\rangle_{\text{GHZ}} &= (-1) |\Psi\rangle_{\text{GHZ}} \\
\hat{\sigma}^A_y \hat{\sigma}^B_y \hat{\sigma}^C_x |\Psi\rangle_{\text{GHZ}} &= (-1) |\Psi\rangle_{\text{GHZ}}
\end{align*}
\]

Hence in HVT the three quantities \( \sigma^A_x \sigma^B_y \sigma^C_z, \sigma^A_y \sigma^B_y \sigma^C_y \) and \( \sigma^A_y \sigma^B_y \sigma^C_x \) must all have value \(-1\) in the GHZ state, so that as the values for these quantities are just the products of the values for each of the factors we get three equations

\[
M^A_x M^B_y M^C_y = -1 \quad M^A_y M^B_x M^C_y = -1 \quad M^A_y M^B_y M^C_x = -1
\]

Secondly, if we apply all three operators \( \hat{\sigma}^A_x \hat{\sigma}^B_x \hat{\sigma}^C_x \) to the GHZ state we find another eigenvalue equation

\[
\hat{\sigma}^A_x \hat{\sigma}^B_x \hat{\sigma}^C_x |\Psi\rangle_{\text{GHZ}} = (+1) |\Psi\rangle_{\text{GHZ}}
\]

which leads to

\[
M^A_x M^B_x M^C_x = +1
\]

However, if we multiply the three equations in Eq.(35) together and use \((M^K)^2 = +1\) we find that \( M^A_x M^B_y M^C_z = -1 \), in direct contradiction to the last equation. Thus the assignment of hidden variables for all the physical quantities \( \sigma^K_\alpha \) fails to describe the GHZ state. As we will see in the next Subsection, there are tests involving the violation of Bell Inequalities that are satisfied by some entangled states which demonstrate the failure of more general local HVT to describe such states.

### 2.6 Paradoxes

The EPR and Schrodinger Cat paradoxes figured prominently in early discussions about entanglement. Both paradoxes involve composite systems and the
consideration of quantum states which are entangled. Both these paradoxes reflect the conflict between quantum theory, in which the values for physical quantities only take on definite values when measurement occurs and classical theory, in which the values for physical quantities always exist even when measurement is not involved. The latter viewpoint is referred to as realism. Quantum theory is also probabilistic so although the possible outcomes for measuring a physical quantity can be determined prior to measurement, the actual outcome in a given quantum state for the measured outcome is only known as a probability. However, from the realist viewpoint, quantum theory is incomplete and a future theory based around hidden variables would determine the actual values of the physical quantities, as well as the quantum probabilities that particular values will be found via measurement.

Whilst the EPR and Schrodinger Cat paradoxes are of historical interest and have provoked much debate, it was the formulation of the Bell inequalities (which are described in the next SubSection) and the conditions under which they could be violated that provided the first clear case of where the predictions of quantum theory could differ from those of hidden variable theories. It then became possible to carry out actual experiments to distinguish these fundamentally different theories. The actual experimental evidence is consistent with quantum theory and rules out hidden variable theories.

2.6.1 EPR Paradox

In the original version of the EPR paradox Einstein et al considered a two-particle system $A$, $B$ in which the particles were associated with positions $\hat{x}_A$, $\hat{x}_B$ and momenta $\hat{p}_A$, $\hat{p}_B$. They envisaged a quantum state in which the pairs of physical quantities $\hat{x}_A$, $\hat{x}_B$ or $\hat{p}_A$, $\hat{p}_B$ had highly correlated values - measured or otherwise. To be specific, one may consider a simultaneous eigenstate of the two commuting operators $\hat{x}_A - \hat{x}_B$ and $\hat{p}_A + \hat{p}_B$, where $(\hat{x}_A - \hat{x}_B)\langle \Phi \rangle = 2x\langle \Phi \rangle$ and $(\hat{p}_A + \hat{p}_B)\langle \Phi \rangle = 0\langle \Phi \rangle$. Thus if $A$ had a mean momentum $p$ then $B$ would have a mean momentum $-p$. Alternatively, if $A$ had a mean position $x$ then $B$ would have a mean position $-x$. Then if the eigenvalue $2x$ is very large the two particles will be well-separated (in quantum theory their spatial wave functions would be localised in separate spatial regions) so that if the position of $B$ was measured then the position of $A$ would be immediately known, even if the particles were light years apart. If the momentum of $B$ was measured instead then the momentum of $A$ would immediately be known. From the realist point of view both $A$ and $B$ always have definite positions and momenta, even if these are not known. It would seem then that measurements of position and momentum on particle $B$ would lead to a knowledge of the position and momentum at a far distant particle $A$, perhaps with an accuracy that would violate the Heisenberg Uncertainty Principle (HUP). Alternatively, the position of $B$ might be measured along with the momentum of $A$, these being commuting observables. But as we have seen, knowing the position of $B$ leads to a knowledge of the position at far-distant particle $A$, so the outcome is that both the position and momentum of $A$ are known, again with the possibility of violating the HUP.
Thus a somewhat paradoxical situation would seem to arise. Einstein stated that this did not demonstrate that quantum theory was wrong, only that it was incomplete.

Discussions of the EPR paradox\(^{11}\) in terms of hidden variable theories has been given by numerous authors (see \([9], [8], [54], [10]\) for example). The recent papers and reviews by Reid et al give a full account taking into consideration the “fuzzy” version of HVT and determining the predictions for the conditional variances for \(x_A\) and \(p_A\) based both on separable quantum states and states described via HVT. This treatment successfully quantifies the somewhat qualitative considerations described in the previous paragraph. If the position for particle \(B\) is measured and the result is \(x\), then the original density operator \(\hat{\rho}\) for the two particle system is changed into the conditional density operator \(\hat{\rho}_{\text{cond}}(\hat{x}_B, x) = \hat{\Pi}_x^B \hat{\rho} \hat{\Pi}_x^B / Tr(\hat{\Pi}_x^B \hat{\rho})\), where \(\hat{\Pi}_x^B = \langle x \rangle_B\) is the projector onto the eigenvector \(|x\rangle_B\) (the eigenvalues \(x\) are assumed for simplicity to form a quasi-continuum). Similarly, if the momentum for particle \(B\) is measured and the result is \(p\), then the original density operator \(\hat{\rho}\) for the two particle system is changed into the conditional density operator \(\hat{\rho}_{\text{cond}}(\hat{p}_B, p) = \hat{\Pi}_p^B \hat{\rho} \hat{\Pi}_p^B / Tr(\hat{\Pi}_p^B \hat{\rho})\), where \(\hat{\Pi}_p^B = \langle p \rangle_B\) is the projector onto the eigenvector \(|p\rangle_B\) (the eigenvalues \(p\) are assumed for simplicity to form a quasi-continuum). Here we outline the discussion based on quantum separable states.

For separable states the conditional probability that measurement of \(\hat{x}_A\) on sub-system \(A\) leads to eigenvalue \(x_A\) given that measurement of \(\hat{x}_B\) on sub-system \(B\) leads to eigenvalue \(x_B\) is obtained from Eq.\((25)\) as

\[
P(\hat{x}_A, x_A|\hat{x}_B, x_B) = \sum_R P_R \hat{P}_A^R(\mathbf{\hat{x}}_A, x_A) \frac{P_B^R(\hat{x}_B, x_B)}{\sum_R P_R P_B^R(\hat{x}_B, x_B)}
\]

(38)

where

\[
P_A^R(\mathbf{\hat{x}}_A, x_A) = Tr_A(\hat{\Pi}_{x_A}^A \hat{\rho}_R) \quad P_B^R(\hat{x}_B, x_B) = Tr_B(\hat{\Pi}_{x_B}^B \hat{\rho}_R)
\]

(39)

are the probabilities for position measurements in the separate sub-systems. The probability that measurement of \(\hat{x}_B\) on sub-system \(B\) leads to eigenvalue \(x_B\) is

\[
P(\hat{x}_B, x_B) = \sum_R P_R P_B^R(\hat{x}_B, x_B)
\]

(40)

The mean result for measurement of \(\hat{x}_A\) for this conditional measurement is from Eq.\((17)\)

\[
\langle \hat{x}_A \rangle_{\hat{x}_B, x_B} = \sum_{x_A} x_A P(\hat{x}_A, x_A|\hat{x}_B, x_B)
\]

\[
= \sum_R P_R \langle \hat{x}_A \rangle_R P_B^R(\hat{x}_B, x_B) / P(\hat{x}_B, x_B)
\]

(41)

where

\[
\langle \hat{x}_A \rangle_R = \sum_{x_A} x_A P_A^R(\mathbf{\hat{x}}_A, x_A)
\]

(42)
is the mean result for measurement of \( \hat{x}_A \) when the sub-system is in state \( \rho_R^A \).

The conditional variance for measurement of \( \hat{x}_A \) for the conditional measurement of \( \hat{x}_B \) on sub-system \( B \) which led to eigenvalue \( x_B \) is from Eq. (15)

\[
\langle \Delta x_A^2 \rangle_{\hat{x}_B,x_B} = \sum_{x_B} (x_A - \langle \hat{x}_A \rangle_{\hat{x}_B,x_B})^2 P(\hat{x}_A|x_B) \\
= \sum_{x_B} P_R \langle \Delta x_A^2 \rangle_{\hat{x}_B,x_B}^R P_B(\hat{x}_B,x_B)/P(\hat{x}_B,x_B) \tag{43}
\]

where

\[
\langle \Delta x_A^2 \rangle_{\hat{x}_B,x_B}^R = \sum_{x_A} (x_A - \langle \hat{x}_A \rangle_{\hat{x}_B,x_B})^2 P_A(\hat{x}_A,x_A)
\]

is a variance for measurement of \( \hat{x}_A \) for when the sub-system is in state \( \rho_R^A \) but now with the fluctuation about the mean \( \langle \hat{x}_A \rangle_{\hat{x}_B,x_B} \) for measurements conditional on measuring \( \hat{x}_B \).

However, for each sub-system state \( R \) the quantity \( \langle \Delta x_A^2 \rangle_{\hat{x}_B,x_B}^R \) is minimised if \( \langle \hat{x}_A \rangle_{\hat{x}_B,x_B} \) is replaced by the unconditioned mean \( \langle \hat{x}_A \rangle_R \) just determined from \( \rho_R^A \). Thus we have an inequality

\[
\langle \Delta x_A^2 \rangle_{\hat{x}_B,x_B} \geq \langle \Delta x_A^2 \rangle^R \tag{44}
\]

where

\[
\langle \Delta x_A^2 \rangle^R = \sum_{x_A} (x_A - \langle \hat{x}_A \rangle^A)^2 P_A(\hat{x}_A,x_A) \tag{45}
\]

is the normal variance for measurement of \( \hat{x}_A \) for when the sub-system is in state \( \rho_R^A \).

Now if the measurements of \( \hat{x}_B \) are unrecorded then the conditioned variance is

\[
\langle \Delta x_A^2 \rangle_{\hat{x}_B} = \sum_{x_B} \langle \Delta x_A^2 \rangle_{\hat{x}_B,x_B} P(\hat{x}_B,x_B) \\
= \sum_{x_B} \sum_{R} P_R \langle \Delta x_A^2 \rangle_{\hat{x}_B,x_B}^R P_B(\hat{x}_B,x_B) \tag{46}
\]

which in view of inequality (44) satisfies

\[
\langle \Delta x_A^2 \rangle_{\hat{x}_B} \geq \sum_{x_B} \sum_{R} P_R \langle \Delta x_A^2 \rangle_{\hat{x}_B,x_B}^R P_B(\hat{x}_B,x_B) \\
= \sum_{R} P_R \langle \Delta x_A^2 \rangle^R \tag{47}
\]

using \( \sum_{x_B} P_B(\hat{x}_B,x_B) = 1 \). Thus the variance for measurement of position \( \hat{x}_A \) conditioned on unrecorded measurements for position \( \hat{x}_B \) satisfies an inequality that only depends on the variances for measurements of \( \hat{x}_A \) in the possible sub-system \( A \) states \( \rho_R^A \).
Now exactly the same treatment can be carried out for the variance of momentum $\hat{p}_A$ conditioned on unrecorded measurements of measurements for momentum $\hat{p}_B$. We have with
\[
\langle \Delta^{2} \hat{p}_A \rangle_{\hat{p}_B} \equiv \sum_{p_B} \langle \Delta^{2} \hat{p}_A \rangle_{\hat{p}_B,p_B} P(\hat{p}_B,p_B)
\]
\[
\langle \Delta^{2} \hat{p}_A \rangle_{\hat{p}_B,p_B} = \sum_{p_A} (p_A - \langle \hat{p}_A \rangle_{\hat{p}_B,p_B})^2 P(\hat{p}_A,p_A \mid \hat{p}_B,p_B)
\]
\[
\langle \hat{p}_A \rangle_{\hat{p}_B,p_B} = \sum_{p_A} P(\hat{p}_A,p_A \mid \hat{p}_B,p_B)
\]
the inequality
\[
\langle \Delta^{2} \hat{p}_A \rangle_{\hat{p}_B} \geq \sum_{R} P_R \langle \Delta^{2} \hat{p}_A \rangle^R
\]
with
\[
\langle \Delta^{2} \hat{p}_A \rangle^R = \sum_{p_A} (p_A - \langle \hat{p}_A \rangle_{\hat{p}_B})^2 P^R(\hat{p}_A,p_A)
\]
is the normal variance for measurement of $\hat{p}_A$ for when the sub-system is in state $\hat{p}_R^A$.

We now multiply the two conditional variances, which it is important to note were associated with two different conditioned states based on two different measurements - position and momentum - carried out on sub-system $B$.
\[
\langle \Delta^{2} \hat{x}_A \rangle_{\hat{x}_B} \langle \Delta^{2} \hat{p}_A \rangle_{\hat{p}_B} \geq \sum_{R} P_R \langle \Delta^{2} \hat{x}_A \rangle^R \sum_{S} P_S \langle \Delta^{2} \hat{p}_A \rangle^S
\]
However, from the general inequality in Eq.(264)
\[
\sum_{R} P_R C_R \sum_{R} P_R D_R \geq \left( \sum_{R} P_R \sqrt{C_RD_R} \right)^2
\]
we then have
\[
\langle \Delta^{2} \hat{x}_A \rangle_{\hat{x}_B} \langle \Delta^{2} \hat{p}_A \rangle_{\hat{p}_B} \geq \left( \sum_{R} P_R \sqrt{\langle \Delta^{2} \hat{x}_A \rangle^R \langle \Delta^{2} \hat{p}_A \rangle^R} \right)^2
\]
\[
= \left( \sum_{R} P_R \sqrt{\langle \Delta^{2} \hat{x}_A \rangle^R \times \langle \Delta^{2} \hat{p}_A \rangle^R} \right)^2
\]
But we know from the HUP that for any given state $\hat{p}_R^A$ that $\langle \Delta^{2} \hat{x}_A \rangle^R \langle \Delta^{2} \hat{p}_A \rangle^R \geq \frac{1}{4} \hbar^2$, so for the conditioned variances associated with a separable state
\[
\langle \Delta^{2} \hat{x}_A \rangle_{\hat{x}_B} \langle \Delta^{2} \hat{p}_A \rangle_{\hat{p}_B} \geq \frac{1}{4} \hbar^2
\]
showing that for a separable state the conditioned variances involving position and momentum measurements on sub-system $B$ still satisfy the HUP. Thus if the EPR violations are to occur then the state must be entangled.
In [54] an analogous treatment based on hidden variable theory also shows that the HUP is satisfied for the conditioned variances. The details of this treatment will not be given here, but the formal similarity of expressions for conditional probabilities in HVT and for separable states indicates the steps involved.

An effect related to the EPR paradox is EPR Steering. As we have seen, the measurement of the position for particle \( B \) changes the density operator and consequently the probability distributions for measurements on particle \( A \) will now be determined from the conditional probabilities, such as \( P_{AB}(\hat{x}_A, x_A | \hat{x}_B, x_B) \) or \( P_{AB}(\hat{p}_A, p_A | \hat{x}_B, x_B) \). Thus measurements on \( B \) are said to steer the results for measurements on \( A \). Steering will of course only apply if the measurement results for \( \hat{x}_B \) are recorded, and not discarded. A discussion of EPR Steering (see [10]) is beyond the scope of this article.

### 2.6.2 Schrodinger Cat Paradox

The Schrodinger Cat Paradox [2], [56] relates to composite systems where one sub-system (the cat) is macroscopic and the other sub-system is microscopic (the radioactive atom). Schrodinger envisaged a state in which an alive cat and an undecayed atom existed at an initial time, and because the decayed atom would be associated with a dead cat, the system after a time corresponding to the half-life for radioactive decay would be described in quantum theory via the entangled state

\[
|\Psi\rangle = \frac{1}{\sqrt{2}} (|e\rangle_{\text{Atom}} |\text{Alive}\rangle_{\text{Cat}} + |g\rangle_{\text{Atom}} |\text{Dead}\rangle_{\text{Cat}}) \quad (54)
\]

in an obvious notation. The combined system is in an enclosed box, and opening the box constitutes a measurement on the system. According to quantum theory if the box was opened at this time there would be a probability of \( 1/2 \) of finding the atom undecayed and the cat alive, with the same probability for finding a decayed atom and a dead cat. From the realist viewpoint the cat should be either dead or it should be alive irrespective of whether the box is opened or not, and it is a paradox that in the quantum theory description of the state prior to measurement the cat is in some sense both dead and alive. This paradox is made worse because the cat is a macroscopic system - how could a cat be either dead or alive at the same time, it must be one or the other? From the quantum point of view in which the actual values of physical quantities only appear when measurement occurs, the Schrodinger cat presents no paradox. The two possible values signifying the health of the cat are "alive" and "dead", and these values are found with a probability of \( 1/2 \) when measurement takes place on opening the box, and this would entirely explain the results if such an experiment were to be performed. In recent times, experiments based on a Rydberg atom in a microwave cavity [57] involving states such as (54) have been performed showing that entanglement can occur between macroscopic and microscopic systems, and it is even possible to prepare states analogous to \( \frac{1}{\sqrt{2}} (|\text{Alive}\rangle_{\text{Cat}} + |\text{Dead}\rangle_{\text{Cat}}) \)
in the macroscopic system itself. In such experiments the different macroscopic states are large amplitude coherent states of the cavity mode.

2.7 Bell Inequalities

A key feature of entangled states is that they are associated with violations of *Bell inequalities* \(^3\) and hence can exhibit this particular *non-classical* feature. The Bell inequalities arise in attempts to restore a *classical* interpretation of quantum theory via hidden variable treatments, where actual values are assigned to all measurable quantities - including those which in quantum theory are associated with non-commuting Hermitian operators. In this case we consider two different physical quantities \(\Omega_A\) for sub-system \(A\), which are listed \(A_1, A_2, \text{etc} \), and two \(\Omega_B\) for sub-system \(B\), which are listed \(B_1, B_2, \text{etc} \). The corresponding quantum Hermitian operators \(\hat{\Omega}_A, \hat{\Omega}_B\), etc are \(\hat{A}_1, \hat{A}_2\) and \(\hat{B}_1, \hat{B}_2\). The Bell inequalities involve the mean value \(\langle A_i \times B_j \rangle_{\text{HVT}}\) of the product of observables \(A_i\) and \(B_j\) for subsystems \(A, B\) respectively, for which there are two possible measured values, +1 and −1. In hidden variable theory, the mean values \(\langle A_i \times B_j \rangle_{\text{HVT}}\) are given by

\[
\langle A_i \times B_j \rangle_{\text{HVT}} = \int d\xi P(\xi) \langle A_i(\xi) \rangle \langle B_j(\xi) \rangle
\]  

where \(\langle A_i(\xi) \rangle\) and \(\langle B_j(\xi) \rangle\) are the values assigned to \(A_i\) and \(B_j\) when the hidden variables are \(\xi\), and \(P(\xi)\) is the hidden variable probability distribution function. If the corresponding quantum Hermitian operators are such that their eigenvalues are +1 and −1 - as in the case of Pauli spin operators - then the only possible values for \(\langle A_i(\xi) \rangle\) and \(\langle B_j(\xi) \rangle\) are +1 and −1, since HVT does not conflict with quantum theory regarding allowed values for physical quantities. However, hidden variable theory predicts certain inequalities for the mean values of products of physical quantities for the two sub-systems.

The form given by Clauser et al \(^4\) for *Bell’s inequality* is

\[
|S| \leq 2
\]  

where

\[
S = \langle A_1 \times B_1 \rangle_{\text{HVT}} + \langle A_1 \times B_2 \rangle_{\text{HVT}} + \langle A_2 \times B_1 \rangle_{\text{HVT}} - \langle A_2 \times B_2 \rangle_{\text{HVT}}
\]  

The minus sign can actually be attached to any one of the four terms.

Following the proof of the Bell inequalities in \(^4\) we have

\[
\langle A_2 \times B_1 \rangle_{\text{HVT}} - \langle A_2 \times B_2 \rangle_{\text{HVT}} = \int d\xi P(\xi) \left( \langle A_2(\xi) \rangle \langle B_1(\xi) \rangle - \langle A_2(\xi) \rangle \langle B_2(\xi) \rangle \right)
\]

\[
= \int d\xi P(\xi) \left( \langle A_2(\xi) \rangle \langle B_1(\xi) \rangle (1 \pm \langle A_1(\xi) \rangle \langle B_2(\xi) \rangle) \right)
\]

\[
- \int d\xi P(\xi) \left( \langle A_2(\xi) \rangle \langle B_2(\xi) \rangle (1 \pm \langle A_1(\xi) \rangle \langle B_1(\xi) \rangle) \right)
\]

(58)
Now all the quantities $\langle A_i(\xi) \rangle$, $\langle B_j(\xi) \rangle$ are either +1 or −1, so the expressions $(1 \pm \langle A_1(\xi) \rangle \langle B_2(\xi) \rangle)$ and $(1 \pm \langle A_1(\xi) \rangle \langle B_1(\xi) \rangle)$ are never negative. Taking the modulus of the left side leads to an equality

$$
|\langle A_2 \times B_1 \rangle_{HVT} - \langle A_2 \times B_2 \rangle_{HVT}| 
\leq 
\int d\xi P(\xi) \left( |\langle A_2(\xi) \rangle \langle B_1(\xi) \rangle| (1 \pm \langle A_1(\xi) \rangle \langle B_2(\xi) \rangle) + |\langle A_1(\xi) \rangle \langle B_2(\xi) \rangle| (1 \pm \langle A_1(\xi) \rangle \langle B_1(\xi) \rangle) \right)
+ \int d\xi P(\xi) \left( |\langle A_2(\xi) \rangle \langle B_2(\xi) \rangle| (1 \pm \langle A_1(\xi) \rangle \langle B_1(\xi) \rangle) + |\langle A_1(\xi) \rangle \langle B_1(\xi) \rangle| (1 \pm \langle A_1(\xi) \rangle \langle B_2(\xi) \rangle) \right)
= 
2 \pm \left( \int d\xi P(\xi) \langle A_1(\xi) \rangle \langle B_2(\xi) \rangle + \int d\xi P(\xi) \langle A_1(\xi) \rangle \langle B_1(\xi) \rangle \right)
= 
2 \pm (\langle A_1 \times B_2 \rangle_{HVT} + \langle A_1 \times B_1 \rangle_{HVT}) \tag{59}
$$

Hence since $|\langle A_1 \times B_2 \rangle_{HVT} + \langle A_1 \times B_1 \rangle_{HVT}| = +(\langle A_1 \times B_2 \rangle_{HVT} + \langle A_1 \times B_1 \rangle_{HVT})$ or $-(\langle A_1 \times B_2 \rangle_{HVT} + \langle A_1 \times B_1 \rangle_{HVT})$ we have

$$
|\langle A_2 \times B_1 \rangle_{HVT} - \langle A_2 \times B_2 \rangle_{HVT}| \leq \langle A_1 \times B_2 \rangle_{HVT} + \langle A_1 \times B_1 \rangle_{HVT} \leq 2 \tag{60}
$$

But since $|X - Y| \leq |X| + |Y|$ we see that from the + version of the last inequality that

$$
|\langle A_2 \times B_1 \rangle_{HVT} - \langle A_2 \times B_2 \rangle_{HVT} + \langle A_1 \times B_2 \rangle_{HVT} + \langle A_1 \times B_1 \rangle_{HVT}| \leq 2 \tag{61}
$$

This is a Bell inequality. Interchanging $A_2 \leftrightarrow A_1$ and repeating the derivation gives $|\langle A_1 \times B_1 \rangle_{HVT} - \langle A_1 \times B_2 \rangle_{HVT} + \langle A_2 \times B_2 \rangle_{HVT} + \langle A_2 \times B_1 \rangle_{HVT}| \leq 2$, which is another Bell inequality. Interchanging $B_1 \leftrightarrow B_2$ and repeating the derivation gives $|\langle A_2 \times B_2 \rangle_{HVT} - \langle A_2 \times B_1 \rangle_{HVT} + \langle A_1 \times B_1 \rangle_{HVT} + \langle A_1 \times B_2 \rangle_{HVT}| \leq 2$, and interchanging $A_2 \leftrightarrow A_1$ and $B_1 \leftrightarrow B_2$ and repeating the derivation gives $|\langle A_1 \times B_2 \rangle_{HVT} - \langle A_1 \times B_1 \rangle_{HVT} + \langle A_2 \times B_1 \rangle_{HVT} + \langle A_2 \times B_2 \rangle_{HVT}| \leq 2$. Thus the minus sign can be attached to any one of the four terms.

### 2.7.1 Non-Entangled State Result

It can be shown that the Bell inequalities also always occur for non-entangled states (see Section 7.3 of the book by Vedral [5]). For Bell’s inequalities we consider Hermitian operators $\hat{A}_i$ and $\hat{B}_j$ for subsystems $A$, $B$ respectively, for which there are two eigenvalues +1 and −1, where examples of the operators are given by the components $\hat{A}_i = a_i \cdot \hat{\sigma}_A$ and $\hat{B}_j = b_j \cdot \hat{\sigma}_B$ of Pauli spin operators $\hat{\sigma}_A$ and $\hat{\sigma}_B$ along directions with unit vectors $a_i$ and $b_j$. The corresponding quantum theory quantity for the Bell inequality is

$$
S = E(\hat{A}_1 \otimes \hat{B}_1) + E(\hat{A}_1 \otimes \hat{B}_2) + E(\hat{A}_2 \otimes \hat{B}_1) - E(\hat{A}_2 \otimes \hat{B}_2) \tag{62}
$$

where in quantum theory the mean value is given by $E(\hat{A}_1 \otimes \hat{B}_j) = \langle \hat{A}_i \otimes \hat{B}_j \rangle = Tr(\rho \hat{A}_i \otimes \hat{B}_j)$. For the general bipartite non-entangled state given by $\rho$ it is
easy to show that

\[ S = \sum_R P_R \left( \langle \hat{A}_1 \rangle_R A \langle \hat{B}_1 + \hat{B}_2 \rangle_R + \langle \hat{A}_2 \rangle_R A \langle \hat{B}_1 - \hat{B}_2 \rangle_R \right) \]  \hspace{1cm} (63)

where \( \langle \hat{A}_1 \rangle_R = Tr(\hat{A}_1 \hat{\rho}_R) \) and \( \langle \hat{B}_j \rangle_R = Tr(\hat{B}_j \hat{\rho}_R) \) are the expectation values of \( \hat{A}_1 \) and \( \hat{B}_j \) for the sub-systems \( A, B \) in states \( \hat{\rho}_R^A \) and \( \hat{\rho}_R^B \) respectively. Now \( \langle \hat{A}_1 \rangle_R \) and \( \langle \hat{B}_j \rangle_R \) must lie in the range \(-1 \) to \(+1 \), so that \( \langle \hat{B}_1 \pm \hat{B}_2 \rangle_R \) must each lie in the range \(-2 \) to \(+2 \). Hence

\[ |S| \leq \sum_R P_R \left( |\langle \hat{A}_1 \rangle_R| |\langle \hat{B}_1 + \hat{B}_2 \rangle_R| + |\langle \hat{A}_2 \rangle_R| |\langle \hat{B}_1 - \hat{B}_2 \rangle_R| \right) \]

\[ \leq \sum_R P_R \left( |\langle \hat{B}_1 + \hat{B}_2 \rangle_R| + |\langle \hat{B}_1 - \hat{B}_2 \rangle_R| \right) \]

\[ \leq 2 \]  \hspace{1cm} (64)

since to obtain \( |\langle \hat{B}_1 + \hat{B}_2 \rangle_R| = 2 \) requires \( \langle \hat{B}_1 \rangle_R = \langle \hat{B}_2 \rangle_R = \pm 1 \) and then

\[ |\langle \hat{B}_1 - \hat{B}_2 \rangle_R| = |\langle \hat{B}_1 \rangle_R - \langle \hat{B}_2 \rangle_R| = 0, \]

or to obtain \( |\langle \hat{B}_1 - \hat{B}_2 \rangle_R| = 2 \) requires \( \langle \hat{B}_1 \rangle_R = -\langle \hat{B}_2 \rangle_R = \pm 1 \) and then \( |\langle \hat{B}_1 + \hat{B}_2 \rangle_R| = |\langle \hat{B}_1 \rangle_R + \langle \hat{B}_2 \rangle_R| = 0. \)

2.7.2 Bell Inequality Violation and Entanglement

It follows that for a general two mode non-entangled state \( |S| \) cannot violate the Bell inequality limit of \( 2 \). Thus, the violation of Bell inequalities proves that the quantum state must be entangled for the sub-systems involved, so Bell inequality violations are a test of entanglement. For entangled states such as the one boson Bell state \( |\Psi_-\rangle \) (see [9], Section 2.5)

\[ |\Psi_-\rangle = \frac{1}{\sqrt{2}} (|0\rangle_A \otimes |1\rangle_B - |1\rangle_A \otimes |0\rangle_B) \]  \hspace{1cm} (65)

the Bell inequality can be violated for the choice where \( a_1, a_2 \) and \( b_1, b_2 \) are orthogonal and \( a_1, a_2 \) are parallel to \( b_1 - b_2, b_1 + b_2 \) respectively (see [9], Section 5.1). Furthermore, such a quantum state cannot be described via a hidden variable theory, since Bell inequalities are always satisfied using a hidden variable theory. Experiments have been carried out in optical systems providing strong evidence for the existence of quantum states that violate Bell inequalities (see [15] for references to experiments). Such violation of Bell inequalities is clearly a non-classical feature, since the experiments rule out hidden variable theory. As Bell inequalities do not occur for separable states, the experimental observation of a Bell inequality indicates the presence of an entangled state.
2.8 Non-local Correlations

Another feature of entangled states is that they are associated with *strong correlations* for observables associated with *localised sub-systems* that are well-separated, a particular example being *EPR correlations* between non-commuting observables. Entangled states can exhibit this particular *non-classical* feature, which again cannot be accounted for via a hidden variable theory.

2.8.1 Hidden Variable Theory

Consider two operators $\hat{\Omega}_A$ and $\hat{\Omega}_B$ associated with sub-systems $A$ and $B$. These would be Hermitian if observables are involved, but for generality this is not required. In a hidden variable theory these would be associated with functions $\Omega_C(\xi)\ (C = A, B)$ of the hidden variables $\xi$, with the Hermitean adjoints $\hat{\Omega}_C^\dagger$ being associated with the complex conjugates $\Omega_C^*(\xi)$. In hidden variable theory *correlation functions* are given by the following mean values

\[
\langle \Omega_A^* \times \Omega_B^HVT = \int d\xi \ P(\xi) \ \Omega_A(\xi) \Omega_B(\xi)
\]

\[
\langle \Omega_A^* \Omega_A \times \Omega_B^\dagger \Omega_B^HVT = \int d\xi \ P(\xi) \ \Omega_A(\xi) \ \Omega_A(\xi) \ \Omega_B^*(\xi) \Omega_B(\xi) \ (66)
\]

satisfy the following *correlation inequality*

\[
| \langle \Omega_A^* \times \Omega_B \rangle^HVT |^2 \leq \langle \Omega_A^* \Omega_A \times \Omega_B^\dagger \Omega_B \rangle^HVT
\]

This result is based on the inequality

\[
\int d\xi \ P(\xi) \ C(\xi) \geq \left( \int d\xi \ P(\xi) \ C(\xi) \right)^2 \quad (68)
\]

for real, positive functions $C(\xi), P(\xi)$ and where $\int d\xi \ P(\xi) = 1$, and which is proved in Appendix 10. In the present case we have $C(\xi) = \Omega_A^*(\xi) \Omega_A(\xi) \ \Omega_B^*(\xi) \Omega_B(\xi)$, which is real, positive. A violation of the inequality in Eq. (67) is an indication of strong correlation between sub-systems $A$ and $B$.

2.8.2 Non-Entangled State Result

It can be shown that the correlation inequalities are *always* satisfied for non-entangled states. In quantum theory the correlation functions are given by

\[
\langle \hat{\Omega}_A^I \otimes \hat{\Omega}_B \rangle = Tr(\hat{\rho} \hat{\Omega}_A^I \otimes \hat{\Omega}_B) \quad \text{and} \quad \langle \hat{\Omega}_A^I \hat{\Omega}_A \otimes \hat{\Omega}_B^I \hat{\Omega}_B \rangle = Tr(\hat{\rho} \hat{\Omega}_A^I \hat{\Omega}_A \otimes \hat{\Omega}_B^I \hat{\Omega}_B).
\]

For a non-entangled state of sub-systems $A$ and $B$ we have

\[
\langle \hat{\Omega}_A^I \otimes \hat{\Omega}_B \rangle = \sum_R P_R \ \langle \hat{\Omega}_A^I \rangle_R^A \ \langle \hat{\Omega}_B \rangle_R^B
\]

\[
\langle \hat{\Omega}_A^I \hat{\Omega}_A \otimes \hat{\Omega}_B^I \hat{\Omega}_B \rangle = \sum_R P_R \ \langle \hat{\Omega}_A^I \hat{\Omega}_A \rangle_R^A \ \langle \hat{\Omega}_B^I \hat{\Omega}_B \rangle_R^B \quad (69)
\]
Now
\[ |\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle| \leq \sum_R P_R |\langle \hat{\Omega}_A^\dagger \rangle_R^A| |\langle \hat{\Omega}_B \rangle_R^B| \quad (70) \]
since the modulus of a sum is always less than the sum of the moduli. Using
\[ \langle \left( \hat{\Omega}_C^\dagger - \langle \hat{\Omega}_C^\dagger \rangle \right) \left( \hat{\Omega}_C - \langle \hat{\Omega}_C \rangle \right) \rangle \geq 0 \] with \((C = A, B)\), we obtain the Schwarz inequality - which is true for all states -
\[ |\langle \hat{\Omega}_C^\dagger \hat{\Omega}_C \rangle| \geq |\langle \hat{\Omega}_C \rangle| = |\langle \hat{\Omega}_C^\dagger \rangle|^2 \]
thus
\[ |\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle| \leq \sum_R P_R \sqrt{\langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \rangle_R^A} \sqrt{\langle \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle_R^B} \quad (71) \]
Next we use the inequality
\[ \sum_R P_R C_R \geq \left( \sum_R P_R \sqrt{C_R} \right)^2 \quad (72) \]
for real, positive functions \(C_R, P_R\) and where \(\sum_R P_R = 1\). This inequality, which was used in the paper by Hillery et al. [32], is proved in Appendix 10. In the present case we have
\[ C_R = \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \rangle_R^A \langle \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle_R^B \]
so that
\[ |\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle|^2 \leq \sum_R P_R \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \rangle_R^A \langle \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle_R^B = \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle \quad (73) \]
Thus for a non-entangled state we obtain the correlation inequality
\[ |\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle|^2 = |\langle \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \rangle|^2 \leq \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle \quad (74) \]
where the general result \(\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle = \langle \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \rangle^*\) has been used. Thus non-entangled states have correlation functions that are consistent with hidden variable theory.

2.8.3 Weak Correlation Violation and Entanglement

Hence if it is found that the correlation inequality is violated \(|\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle|^2 = |\langle \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \rangle|^2 > \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle\) then the state must be entangled, so the correlation inequality violation is also a test for entanglement. Again entangled states have features that cannot be explained via hidden variable theory, so entangled states are clearly non-classical. ..
2.9 Identical Particles - Symmetrisation Principle

2.9.1 Symmetrization and Second Quantization

Whether entangled or not the physical states for systems of identical particles must conform to the symmetrisation principle, whereby the overall density operator has to be invariant under permutation operators. Problems arise regarding how to define non-entangled states for systems of identical particles. The basic issue is how first to distinguish what are meaningful sub-systems for identical particle systems. Some authors ([45], [58],..) consider states of the form

\[ \hat{\rho} = \sum_R P_R \hat{\rho}_R^1 \otimes \hat{\rho}_R^2 \otimes \hat{\rho}_R^3 \otimes ... \] (75)

to be non-entangled states, where \( \hat{\rho}_R^i \) is a density operator for particle \( i \). However such a state would not in general be physical, since the symmetrisation principle would be violated unless the \( \hat{\rho}_R^i \) were related. For example, consider the state for two identical bosonic atoms given by

\[ \hat{\rho} = P_{\sigma \xi} \hat{\sigma}^1 \otimes \hat{\xi}^2 + P_{\theta \eta} \hat{\theta}^1 \otimes \hat{\eta}^2 \] (76)

and apply the permutation \( \hat{P} = \hat{P}(1 \leftrightarrow 2) \). The invariance of \( \hat{\rho} \) in general requires \( \hat{\sigma} = \hat{\xi} \) and \( \hat{\theta} = \hat{\eta} \), giving \( \hat{\rho} = P_{\sigma \xi} \hat{\sigma}^1 \otimes \hat{\sigma}^2 + P_{\theta \eta} \hat{\theta}^1 \otimes \hat{\theta}^2 \). This is a statistical mixture of two states, one with both atoms in state \( \hat{\sigma} \), the other with atoms in state \( \hat{\theta} \). Of course if the atoms were all different (atom 1 a Rb\(^{87}\) atom, atom 2 a Na\(^{23}\) atom,..) then the expression (76) would be a valid non-entangled state, but there the atomic sub-systems are distinguishable and symmetrisation is not required. What is distinguishable for systems of identical bosons is not the individual particles themselves - which do not carry labels, boson 1, boson 2, etc. - but the single particle states or modes that the bosons may occupy. For bosonic atoms with several hyperfine components, each component will have its own set of modes. The same would apply to fermionic atoms. For photons the modes may be specified via wave vectors and polarisations. Although the quantum pure states can be specified via symmetrized products of single particle states occupied by specific particles using a first quantization approach, it is more convenient to use second quantization. Here, a basis set for the quantum states of such sub-systems are the Fock states \( |n_a\rangle \) \( (n_a = 0, 1, 2,..) \) etc, which specify the number of identical particles occupying the mode \( A \), etc., so in this approach the mode is the sub-system and the Fock states give different physical states for this sub-system. Symmetrization is built into the definition of the Fock states. If the atoms were fermions rather than bosons the Pauli exclusion principle would of course restrict \( n_a = 0, 1 \) only. Thus in this second quantization approach situations with differing numbers of identical particles are different states, not different systems. The overall system will be associated with physical states with density operators and state vectors in Fock space, which includes states with total numbers of identical particles ranging from zero in the vacuum state right up to infinity.
2.9.2 Sub-Systems and Modes

The point of view in which the possible sub-systems $A$, $B$, etc are modes (or sets of modes) rather than particles has been adopted by several authors ([12], [13], [14]), [8], [22], [23] and will be the approach used here. What are or are not entangled are modes not particles. Overall, the system is a collection of modes, not particles. Particles are associated with mode occupancies, and therefore related to specifying the quantum states of the system, rather than the system itself. Note that in this approach states where there is only a single atom may still be entangled states - for example with two spatial modes $A,B$ the states which are a quantum superposition of the atom in each of these modes, such as the Bell state $(|1_a⟩|0_b⟩ + |0_a⟩|1_b⟩)/\sqrt{2}$ are entangled states. For entangled states associated with the EPR paradox or for quantum teleportation, the mode functions may be localised in well-separated spatial regions - spooky action at a distance - but spatially overlapping mode functions apply in other situations. Furthermore, as well as being distinguishable the modes can act as separate systems, with other modes being ignored. For interacting bosonic atoms this is much harder to accomplish experimentally than for the case of photons, where the relatively slow processes in which photons are destroyed in one EM field mode and created in another may require the presence of atoms as intermediaries. Two bosonic atoms in one mode may collide rapidly disappear into other modes. However, atomic boson interactions can be made very small via Feshbach resonance methods. Near absolute zero the basic physics of a BEC in a single trap potential is describable via a one mode theory. Hence with $A, B, ..$ signifying distinct modes, the general non-entangled state is given in Eq. though the present paper mainly involves only two modes.

It is useful to clarify the meaning of entanglement used in the present paper via a simple example. Consider a situation in which there are two distinct single particle states (modes) designated as $|u⟩$ and $|v⟩$. These states are chosen to be orthogonal. We consider a system with $N = 2$ particles, which may be identical and are labeled 1 and 2, or they may be distinguishable and labeled $\alpha$ and $\beta$.

For the case of the identical particles we consider pure states for two bosons and for two fermions, which are written in terms of first quantization as

$$|\Psi\rangle_{boson} = \frac{1}{\sqrt{2}}(|u(1)⟩ \otimes |v(2)⟩ + |v(1)⟩ \otimes |u(2)⟩)$$  \hspace{1cm} (77)

$$|\Psi\rangle_{fermion} = \frac{1}{\sqrt{2}}(|u(1)⟩ \otimes |v(2)⟩ - |v(1)⟩ \otimes |u(2)⟩)$$  \hspace{1cm} (78)

and clearly satisfy the symmetrization principle. The question is: are these entangled states? They certainly look entangled because both are sums of the products of two state vectors. In the textbook by Peres ([6], see pp126-128) it is stated that ”two particles of the same type are always entangled”. Peres obviously considers such entanglement is a result of symmetrization. However, noting that there is only one type of particle involved and there are two modes that can be occupied, in second quantization the state in both the fermion and...
bouon cases is

$$|\Psi\rangle = |1\rangle_u \otimes |1\rangle_v$$

(79)

which is a separable state for modes $u, v$, and not a (mode) entangled state. On the other hand, the boson state $(|u(1)\rangle \otimes |u(2)\rangle + |v(1)\rangle \otimes |v(2)\rangle)/\sqrt{2}$ is an entangled state, written in second quantization as $(|2\rangle_u \otimes |0\rangle_v + |0\rangle_u \otimes |2\rangle_v)/\sqrt{2}$.

There is no analogous state for fermions due to the Pauli principle.

Now consider the case where the particles are distinguishable. Pure states analogous to the previous ones are given in first quantization as

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|u(\alpha)\rangle \otimes |v(\beta)\rangle \pm |v(\alpha)\rangle \otimes |u(\beta)\rangle)$$

(80)

which are not required to satisfy the symmetrization principle since the particles are not identical. Each may be either a boson or a fermion. The question is: are these entangled states? Noting that for each particle there are two modes that could be occupied, in second quantization the state would be written as

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle_u \otimes |0\rangle_v)_{\alpha} \otimes (|0\rangle_u \otimes |1\rangle_v)_{\beta} \pm (|0\rangle_u \otimes |1\rangle_v)_{\alpha} \otimes (|1\rangle_u \otimes |0\rangle_v)_{\beta}$$

(81)

These are both entangled states.

It is worth noting that these examples illustrate the general point that just the mathematical form of the state vector or the density operator alone is not enough to determine whether a separable or an entangled state is involved. The meaning of the factors involved also has to be taken into account. Failure to realise this may lead to states being regarded as separable which should not be (see SubSection 2.12 for further examples). In the case just presented involving a system with two particles, the quantities $|u(1)\rangle$ or $|v(2)\rangle$ do not specify valid sub-system states when the particles are identical, so the forms given by (77) and (78) do not represent entangled states. On the other hand, the quantities $|u(\alpha)\rangle$ or $|v(\beta)\rangle$ do specify valid sub-system states when the particles are distinguishable, so the forms given by (80) do represent entangled states.

The approach of Wiseman et al [20] to defining an entanglement measure in the case of identical particle systems seems to be completely compatible with the entanglement definition used in the present paper. The identical particles are divided between two observers $A$ and $B$, and a general $N$ particle normalised pure state $|\Psi_{AB}\rangle$ for the overall system is considered. A so-called entropy of particle entanglement is defined via the expression $E_P(|\Psi_{AB}\rangle) = \sum_n P_n E_M(|\Psi_{AB}^{(n)}\rangle)$, where $|\Psi_{AB}^{(n)}\rangle = \sum_n \Pi_n |\Psi_{AB}\rangle$ (un-normalised) is the state $|\Psi_{AB}\rangle$ projected onto the sub-space where there are $n$ identical particles associated with $A$ and $N - n$ with $B$. $P_n$ is the probability that there will be $n$ particles associated with $A$, given by $P_n = Tr(\sum \Pi_n |\Psi_{AB}\rangle \langle \Psi_{AB}|)$. The (mode) entropy for the state $|\Psi_{AB}^{(n)}\rangle$ is $E_M(|\Psi_{AB}^{(n)}\rangle) = S(\hat{\rho}_{AB}^n)$ where $S(\hat{\rho}) = -Tr(\hat{\rho} \log_2 \hat{\rho})$ is the von Neumann entropy and $\hat{\rho}_{AB}^n = Tr_B(|\Psi_{AB}^{(n)}\rangle \langle \Psi_{AB}^{(n)}|) / \langle \Psi_{AB}^{(n)}| \Psi_{AB}^{(n)}\rangle$ is the density operator for
s are sets of modes. As in the previous example, each mode pair is associated with Heaney et al [60], again involving four modes associated with a double well potential well are considered (see Subsection 5.6). A further example is treated

Entanglement criteria for the mode pairs based on local spin operators associated with each potential well are considered (see Subsection 5.3). For completeness a brief description of orthonormal states as

The most general pure state could always be written in terms of orthonormal states as

where

is a normalised n particle state for sub-system A and

is a normalised N − n particle state for sub-system B. For such a separable state of sub-systems A and B

is non-zero the entropy of particle entanglement is zero, so as would be expected. The most general pure state could always be written in terms of orthonormal states as

where

If more than one

is non-zero, then

if more than one

is non-zero the entropy of particle entanglement is non-zero, so Wiseman et al would regard this general state as entangled, just as we do. In this paper no quantitative measure of entanglement has been specifically proposed, so the entropy of particle entanglement proposed by Wiseman et al [20] is consistent with our work.

Note however that a different concept of entanglement - particle entanglement - has also been applied to identical particle systems [43]. This is not the same as mode entanglement so tests and measures for particle entanglement will differ from those for mode entanglement. For completeness a brief description highlighting the difference between mode and particle entanglement is presented in Appendix [11]. A further discussion about the distinction is given in [19].

2.9.3 Multi-Mode Sub-Systems

As well as the simple case where the sub-systems are all individual modes, the concept of entanglement may be extended to situations where the sub-systems are sets of modes, rather than individual modes. In this case entanglement or non-entanglement will be of these distinct sets of modes. Such a case in considered in Subsection [5.3] where pairs of modes associated with distinct lattice sites are considered as the sub-systems. Another example is treated in He et al [59], which involves a double well potential with each well associated with two bosonic modes, these pairs of modes being the two sub-systems. Entanglement criteria for the mode pairs based on local spin operators associated with each potential well are considered (see Subsection 5.3). A further example is treated by Heaney et al [60], again involving four modes associated with a double well potential. As in the previous example, each mode pair is associated with the
same well in the potential, but here a Bell entanglement test was obtained for pairs of modes in the different wells. The concept of *entanglement of sets of modes* is a straightforward extension of the basic concept of entanglement of individual modes.

### 2.10 Super-Selection Rule

#### 2.10.1 Global Particle Number SSR

The question of what physical states - entangled or not - are possible in the non-relativistic quantum physics of a system of identical bosonic particles - such as bosonic atoms or photons - has been the subject of much discussion. Whether entangled or not it is generally accepted that there is a super-selection rule that prohibits quantum superposition states of the form

$$|\Phi\rangle = \sum_{N=0}^{\infty} C_N |N\rangle$$

$$\hat{\rho} = \sum_{N=0}^{\infty} |C_N|^2 |N\rangle \langle N| + \sum_{N=0}^{\infty} \sum_{M=0}^{\infty} (1-\delta_{N,M})C_N C_M^* |N\rangle \langle M|$$

being physical states when they involve Fock states $|N\rangle$ with differing total numbers $N$ of particles. The density operator for such a state would involve coherences between states with differing $N$. Although such superpositions - such as the Glauber coherent state $|\alpha\rangle$, where $C_N = \exp(-|\alpha|^2/2)\alpha^N/\sqrt{N!}$ - do have a useful mathematical role, they do not represent actual physical states according to the super-selection rule. The papers by Sanders et al [39] and Cable et al [61] are examples of applying the SSR for optical fields, but also using the mathematical features of coherent states to treat phenomena such as interference between independent lasers. The super-selection rule indicates that the most general physical state for a system of identical bosonic particles can only be of the form

$$\hat{\rho} = \sum_{N=0}^{\infty} \sum_{\Phi} P_{\Phi,N} (|\Phi_N\rangle \langle \Phi_N|)$$

$$|\Phi_N\rangle = \sum_i C_i^N |N\rangle i$$

where $|\Phi_N\rangle$ is a quantum superposition of states $|N\rangle i$ each of which involves exactly $N$ particles, and where different states with the same $N$ are designated as $|N\rangle i$. This state $\hat{\rho}$ is a statistical mixture of states, each of which contains a specific number of particles. Such a SSR is referred to as a global SSR, as it applies to the system as a whole. Mathematically, the global particle number SSR can be expressed as

$$[\hat{N}, \hat{\rho}] = 0$$

where $\hat{N}$ is the total number operator.

#### 2.10.2 Examples of Global Particle Number SSR Compliant States

Examples of a state vector $|\Phi_N\rangle$ for an entangled pure state [13] and a density operator $\hat{\rho}$ for a non-entangled mixed [62] state for a two mode bosonic system,
both of which are possible physical states are

\[ |\Phi_N\rangle = \sum_{k=0}^{N} C(N, k) |k\rangle_A \otimes |N - k\rangle_B \]  

(85)

\[ \hat{\rho} = \sum_{k=0}^{N} P(k) |k\rangle_A \langle k|_A \otimes |N - k\rangle_B \langle N - k|_B \]  

(86)

The entangled pure state is a superposition of product states with \( k \) bosons in mode \( A \) and the remaining \( N - k \) bosons in mode \( B \). Every term in the superposition is associated with the same total boson number \( N \). The non-entangled mixed state is a statistical mixture of product states also with \( k \) bosons in mode \( A \) and the remaining \( N - k \) bosons in mode \( B \). Every term in the statistical mixture is associated with the same total boson number \( N \). For the case of a two mode fermionic system the Pauli exclusion principle restricts the number of possible fermions to two, with at most one fermion in each mode. Expressions for a state with exactly \( N = 2 \) fermions are

\[ |\Phi_2\rangle = |1\rangle_A \otimes |1\rangle_B \]  

(87)

\[ \hat{\rho} = |1\rangle_A \langle 1|_A \otimes |1\rangle_B \langle 1|_B \]  

(88)

Neither state is entangled and both are the same pure state since \( \hat{\rho} = |\Phi_2\rangle \langle \Phi_2| \).

Although the super-selection rules and symmetrisation principle also applies to fermions, as indicated in the Introduction this paper is focused on bosonic systems, and it will be assumed that the modes are bosonic unless indicated otherwise.

The Bell states for \( N = 2 \) bosons provide important examples of four mode pure quantum states that are compliant with the global particle number SSR. The modes are designated \( A+, A-, B+, B- \) and the Fock states are in general \( |n_{A+}, n_{A-}, n_{B+}, n_{B-}\rangle \). The Bell states may be written

\[ |\Psi_{\text{singlet}}\rangle = \frac{1}{\sqrt{2}}(|1, 0, 0, 1\rangle - |0, 1, 1, 0\rangle) \equiv \frac{1}{\sqrt{2}}(|A+\rangle \otimes |B-\rangle - |A-\rangle \otimes |B\rangle) \]

\[ |\Psi_{\text{triplet},+1}\rangle = |1, 0, 1, 0\rangle \equiv |A+\rangle \otimes |B+\rangle \]

\[ |\Psi_{\text{triplet},0}\rangle = \frac{1}{\sqrt{2}}(|1, 0, 0, 1\rangle + |0, 1, 1, 0\rangle) \equiv \frac{1}{\sqrt{2}}(|A+\rangle \otimes |B-\rangle + |A-\rangle \otimes |B\rangle) \]

\[ |\Psi_{\text{triplet},-1}\rangle = |0, 1, 0, 1\rangle \equiv |A-\rangle \otimes |B-\rangle \]  

(89)

where the second forms may be more familiar. Of these states \( |\Psi_{\text{singlet}}\rangle \) and \( |\Psi_{\text{triplet},0}\rangle \) are entangled, whilst \( |\Psi_{\text{triplet},+1}\rangle \) and \( |\Psi_{\text{triplet},-1}\rangle \) are separable.

### 2.10.3 Super-Selection Rules and Conservation Laws

It is important to realise that such super-selection rules are additional constraints to those imposed by conservation laws. For example, the conservation law on total particle number only leads to the requirement on the superposition state \( |\Phi\rangle \) that the \( |C_N|^2 \) are time independent, it does not require only one \( C_N \)
being non-zero. Super-selection rules are broad in their scope, forbidding quantum superpositions of states of systems with differing charge, differing baryon number and differing statistics. Thus a combined system of a hydrogen atom and a helium ion does not exist in quantum states that are linear combinations of hydrogen atom states and helium ion states - the super-selection rules on both charge and baryon number preclude such states. The basis physical states for such a combined system would involve symmetrised tensor products of hydrogen atom and helium ion states, not linear combinations - symmetrisation being required because the system contains two identical electrons. On the other hand, super-selection rules do not prohibit quantum superpositions of states of systems with differing energy, angular or linear momenta - other physical quantities that may also be conserved. Thus in a hydrogen atom quantum superpositions of states with differing energy and angular momentum quantum numbers are allowed physical states.

2.10.4 SSR Justification and No Suitable Phase Reference

There are two types of justification for applying the super-selection rules for systems of identical particles. The first approach is based on simple considerations and will be outlined below in this subsection. The second approach \[37\], \[38\], \[39\], \[40\], \[41\], \[42\], \[31\], \[34\], \[35\], \[17\] is more sophisticated and involves linking the absence or presence of SSR to whether or not there is a suitable reference frame in terms of which the quantum state is described, and is outlined in the next subsection and Appendix \[12\]. The key idea is that SSR are a consequence of considering the description of a quantum state by an external observer (Charlie) whose phase reference frame has an unknown phase difference from that of an observer ((Alice) more closely linked to the system being studied. Thus, whilst Alice’s description of the quantum state may violate the SSR, the description of the same quantum state by Charlie will not. In the main part of this paper the density operator \(\hat{\rho}\) used to describe the various quantum states will be that of the external observer (Charlie).

2.10.5 SSR Justification and Physics Considerations

A number of straightforward reasons have been given in the Introduction for why it is appropriate to apply the superselection rule to exclude quantum superposition states of the form \([82]\) as physical states for systems of identical particles, and these will now be considered in more detail.

Firstly, no way is known for creating such states. The Hamiltonian for such a system commutes with the total boson number operator, resulting in the \(|C_N|^2\) remaining constant, so the quantum superposition state would need to have existed initially. In the simplest case of non-interacting bosonic atoms, the Fock states are also energy eigenstates, such Fock states involve total energies that differ by energies of order the rest mass energy \(mc^2\), so a coherent superposition of states with such widely differing energies would at least seem unlikely in a non-relativistic theory, though for massless photons this would not be an
issue as the energy differences are of order the photon energy $\hbar \omega$. The more important question is: Is there a non-relativistic quantum process could lead to the creation of such a state? Processes such as the dissociation of $M$ diatomic molecules into up to $2M$ bosonic atoms under Hamiltonian evolution involve entangled atom-molecule states of the form

$$|\Phi\rangle = \sum_{m=0}^{M} C_m |M-m\rangle_{\text{mol}} \otimes |2m\rangle_{\text{atom}} \quad (90)$$

but the reduced density operator for the bosonic atoms is

$$\hat{\rho}_{\text{atoms}} = \sum_{m=0}^{M} |C_m|^2 (|2m\rangle \langle 2m|)_{\text{atom}} \quad (91)$$

which is a statistical mixture of states with differing atom numbers with no coherence terms between such states. Such statistical mixtures are valid physical states, corresponding to a lack of a priori knowledge of how many atoms have been produced. To obtain a quantum superposition state for the atoms alone, the atom-molecule state vector would need to evolve at some time into the form

$$|\Phi\rangle = \sum_{m=0}^{M} B_m |M-m\rangle_{\text{mol}} \otimes \sum_{n=0}^{M} A_{2n} |2n\rangle_{\text{atom}} \quad (92)$$

where the separate atomic system is in the required quantum superposition state. However if such a state existed there would be terms with at least one non-zero coefficient $B_m A_{2n}$ involving product states $|M-m\rangle_{\text{mol}} \otimes |2n\rangle_{\text{atom}}$ with $n \neq m$ if the state $|\Phi\rangle$ is not just in the entangled form $(90)$. However, the presence of such a term would mean that the conservation law involving the number of molecules plus two times the number of atoms was violated. This is impossible, so such an evolution is not allowed.

Secondly, no way is known for measuring all the properties of such states, even if they existed. If a state such as $(92)$ did exist then the amplitudes $C_N$ would oscillate with frequencies that differ by relativistic frequencies of order $mc^2/\hbar$, even if boson-boson interactions were included. To distinguish the phases of the $C_N$ in order to verify the existence of the state, measurement operators would need to include terms that also oscillate at relativistic frequencies, and no such measurement operators are known.

Thirdly, there is no need to invoke the existence of such states in order to understand coherence and interference effects. It is sometimes thought that states involving quantum superpositions of number states are needed for discussing coherence and interference properties of BECs, and some papers describe the state via the Glauber coherent states. However, as Leggett [63] has pointed out (see also Bach et al [64], Dalton and Ghanbari [65]), a highly occupied number state for a single mode with $N$ bosons has coherence properties of high order $n$, as long as $n \ll N$. The introduction of a Glauber coherent state is not required to account for coherence effects. Even the well-known presence of spatial interference patterns produced when two independent BECs are overlapped can be
accounted for via treating the BECs as Fock states. The interference pattern is built up as a result of successive boson position measurements [66], [39], [61].

Fourthly, the stability of such states against decoherence processes may not be great, so even if they could be created, they could rapidly change to other states. However, decoherence time scales that are not too short would be acceptable. Although BECs are created in high vacuum experiments and are well isolated from the external environment in magnetic or dipole traps, they are not entirely free from decoherence effects because the bosons do interact with each other. Even in a single mode case boson-boson collisions can cause dephasing effects. These could be shown via the decay of the coherence $\langle \hat{a} \rangle$. However, it may turn out that the lifetime of a coherent state in a single mode BEC is quite long - in the case of photons the lifetime could be as long as the inverse Townes-Schawlow line width, perhaps of order $10^3$ s (see below). If a coherent superposition state could be created with a non-zero coherence, this may last long enough to carry out further experiments, so this fourth reason for discarding coherent superposition states is relatively unimportant though further studies of their lifetimes would be of some theoretical interest.

2.10.6 SSRJustification and Galilean Frames

Finally, in addition to the previous reasons there is an argument based on the requirement that the dynamical equations for such non-relativistic quantum systems should be invariant under a Galilean transformation which has been proposed [67] as a proof of the super-selection rule for atom number. This approach is linked to the reference frame based justification of SSR (see Appendix 12). However, whilst the paper shows that under a Galilean transformation - corresponding to describing the system from the point of view of an observer moving with a constant velocity $v$ with respect to the original observer, and where the two observers have identical clocks - the terms in a superposition state with different numbers $N$ of massive bosons would oscillate like $\exp(i \frac{1}{2} Nmv^2 t)/\hbar$, and may be expected if the same quantum state is described by a moving observer. This feature alone does not seem to require the super-selection rule, since here the moving observer’s reference frame has a well-defined velocity with respect to that attached to the system. However, the moving observer’s reference frame may actually have an unknown relative velocity, in which case a twirling operation resulting in the elimination of number state coherences could be involved (see Appendix 12). This will not be considered further at this stage.

On the other hand, an approach of this kind involving rotation symmetry would seem to rule out such states as quantum superpositions of a boson (spin 0) and a fermion (spin 1/2). Let such a state be prepared in the form $(|F\rangle + |B\rangle)/\sqrt{2}$. Consider an observer whose cartesian reference frame is $X, Y, Z$. This is a classical system that can be rotated in space. If the observer rotates with his frame through $2\pi$ about any axis they are then back in the same position, but the observer now sees the state as $(-|F\rangle + |B\rangle)/\sqrt{2}$. This state is apparently orthogonal to the one observed before the rotation, and this is paradoxical since the observer would be in the same position. Thus there is a super-selection rule
excluding states such as \((|F\rangle + |B\rangle)/\sqrt{2}\). A similar argument based on the time reversal anti-unitary operator was given by Wick et al [30].

### 2.10.7 SSR and Photons

Though this paper is focused on massive bosonic atoms the question is whether similar considerations also apply to the optical quantum EM field, which involve massless bosons - photons. Here the situation is not so clear.

In the case of photons, Mølmer [68] has argued that the physical state for a single mode optical laser field operating well above threshold is not a Glauber coherent state, and the density operator would be a statistical mixture of the form (83), with \(|\Phi_N\rangle = |N\rangle\) and \(P_{\Phi N} = \exp(-\lambda N) N^\lambda /\lambda!\). Here the density operator is a statistical mixture of photon number states with Poisson distribution, or equivalently a statistical mixture of coherent states \(|\alpha\rangle\) with \(\alpha = \sqrt{N} \exp(i\phi)\) and all phases \(\phi\) having equal probability. Some of the same general reasons for applying the super-selection rule to systems of identical massive bosons also apply here, though the details differ. For the free quantum EM field there is a conservation law for the photon number in each mode, so in this case again \(|C_N|^2\) would be time independent. However, for photons the \(C_N\) would oscillate with frequencies that only differ by non-relativistic frequencies of order \(\hbar \omega\), so the argument against coherent states based on this feature do not apply. In terms of preparing states, in the case of the single mode optical laser the field is generated via interactions with incoherently pumped atoms, there is no well defined optical phase that can be imposed on the process, and the quantum theory for such laser processes predicts a quantum state that is a statistical mixture of photon number states. In the case of the optical laser field coherent states are not physical unless there are optical reference fields with a well-defined phase that could be used to determine the phases associated with the expansion coefficients. This may now becoming possible with the development of atomic clocks based on optical atomic transitions that may supercede atomic clocks based on atomic transitions at microwave frequencies. Optical interference and coherence effects can also be explained without invoking Glauber coherent states, as [68] and others such as [39] have shown. However, if coherent states could be created they might be relatively stable. In the optical laser field case, phase loss via diffusion is related to the laser linewidth, and this can be reduced to the Townes-Schawlow limit that varies inversely as the mean photon number - which is large. The Townes-Schawlow linewidth can be as small as \(10^{-3}\) Hz, corresponding to a phase diffusion time of \(10^3\) s. An alternative approach is presented by Wiseman et al [69], [70], in which the optical laser is treated via a master equation, but where monitoring of the laser environment (difficult!) is required to determine whether certain pure state ensembles - such as those involving coherent states - are physically realisable. The conclusion reached is that for finite self energy the coherent state ensemble is not physically realisable, the closest ensemble being that involving squeezed states, though for zero self energy coherent state ensembles are obtained.

Another approach to the question (see next sub-section and SubSection [124])
in Appendix 12 involves the consideration of phase reference frames. The quantum state of a single mode laser may be described as a Glauber coherent state by an observer (Alice) with one reference frame, but would be described as a statistical mixture of photon number states by another observer (Charlie) with a different reference frame whose phase reference is completely unrelated to the previous one. However, this argument against the presence of coherent state in Charlie’s viewpoint would be overcome if phase references at optical frequencies are developed.

2.11 Reference Frames and Violations of Superselection Rules

Challenges to the requirement for physical states to be consistent with super-selection rules have occurred since the 1960’s when Aharonov and Susskind [37] suggested that coherent superpositions of different charge eigenstates could be created. It is argued that super-selection rules are not a fundamental requirement of quantum theory, but the restrictions involved could be lifted if there is a suitable system that acts as a reference for the coherences involved - [37], [38], [39], [40], [41], [42], [31], [34], [35], [17] provide discussions regarding reference systems and SSR.

2.11.1 Linking SSR and Reference Frames

The discussion of the super-selection rule issue in terms of reference systems is quite complex and too lengthy to be covered in the body of this paper. However, in view of the wide use of the reference frame approach a full outline is presented in Appendix 12. The key idea is that there are two observers - Alice and Charlie - who are describing the same quantum state in terms of their own reference systems. The reference systems are macroscopic systems in states where the behaviour is essentially classical, such as large magnets that can be used to define cartesian axes or BEC in Glauber coherent states that are introduced to define a phase reference. The relationship between the two reference systems is represented by a group of unitary transformation operators listed as $\hat{T}(g)$, where the particular transformation (translation or rotation of cartesian axes, phase change of phase references, ..) that changes Alice’s reference system into Charlie’s is denoted by $g$. Alice is the internal observer, closely linked to the system under study and describes the quantum state via her density operator, whereas Charlie is the external observer whose specification of the same quantum state via his density operator is of most interest. There are two cases of importance, Situation A - where the relationship between Alice’s and Charlie’s reference frame is is known and specified by a single parameter $g$, and Situation B - where on the other hand the relationship between frames is completely unknown, all possible transformations $g$ must be given equal weight. Situation A is not associated with SSR, whereas Situation B leads to SSR. The relationship between Alice’s and Charlie’s density operators is given in terms of the transformation operators (see Eq. 273 for Situation A and Eq. 274)
for Situation B). In Situation B there is often a qualitative change between Alice’s and Charlie’s description of the same quantum state, with pure states as described by Alice becoming mixed states when described by Charlie. It is Situation B with the U(1) transformation group - for which number operators are the generators - that is of interest for the single or multi-mode systems involving identical bosons on which the present paper focuses. An example of the qualitative change of behaviour for the single mode case is that if it is assumed that Alice could prepare the system in a Glauber coherent pure state - which involves SSR breaking coherences between differing number states - then Charlie would describe the same state as a Poisson statistical mixture of number states - which is consistent with the operation of the SSR. Thus the SSR applies in terms of external observer Charlie’s description of the state. This is how the dispute on whether the state for single mode laser is a coherent state or a statistical mixture is resolved - the two descriptions apply to different observers - Alice and Charlie. On the other hand there are quantum states such as Fock states and Bell states which are described the same way by both Alice and Charlie, even in Situation B. The general justification of the SSR for Charlie’s density operator description of the quantum state in Situation B is derived in terms of the irreducible representations of the transformation group, there being no coherences between states associated with differing irreducible representations (see Eq. (298)). For the particular case of the U(1) transformation group the irreducible representations are associated with the total boson number for the system or sub-system, hence the SSR that prohibits coherences between states where this number differs. Finally, it is seen that if Alice describes a general non-entangled state of sub-systems - which being separable have their own reference frames - then Charlie will also describe the state as a non-entangled state and with the same probability for each product state (see Eqs. (303) and (304)). For systems involving identical bosons Charlie’s description of the sub-system density operators will only involve density operators that conform to the SSR. This is in accord with the key idea of the present paper.

2.11.2 Coherent Superposition of Atom and Molecule?

Based around the reference frame approach Dowling et al [71] and Terra Cunha et al [14] propose processes using a BEC as a reference system that would create a coherent superposition of an atom and a molecule, or a boson and a fermion [71]. Dunningham et al [72] consider a scheme for observing a superposition of a one boson state and the vacuum state. Obviously if super-selection rules can be overcome in these instances, it might be possible to produce coherent superpositions of Fock states with differing particle numbers such as Glauber coherent states, though states with $N \sim 10^8$ would presumably be difficult to produce. However, detailed considerations of such papers indicate that the states actually produced in terms of Charlie’s description are statistical mixtures consistent with the super-selection rules rather than coherent superpositions, which are only present in Alice’s description of the state. Also, although coherence and interference effects are demonstrated, these can also be accounted for without
invoking the presence of coherent superpositions that violate the super-selection rule. As the paper by Dowling et al. [71] entitled "Observing a coherent superposition of an atom and a molecule." is a good example of where the super-selection rules are challenged, the key points are described in Appendix 13. Essentially the process involves one atom $A$ interacting with a BEC of different atoms $B$ leading to the creation of one molecule $AB$, with the BEC being depleted by one $B$ atom. There are three stages in the process, the first being with the interaction that turns separate atoms $A$ and $B$ into the molecule $AB$ turned on at Feshbach resonance for a time $t$ related to the interaction strength and the mean number of bosons in the BEC reference system, the second being free evolution at large Feshbach detuning $\Delta$ for a time $\tau$ leading to a phase factor $\phi = \Delta \tau$, the third being again with the interaction turned on at Feshbach resonance for a further time $t$. However, it is pointed out in Appendix 13 that Charlie’s description of the state produced for the atom plus molecule system is merely a statistical mixture of a state with one atom and no molecules and a state with no atom and one molecule, the mixture coefficients depending on the phase $\phi$ imparted during the process. However a coherent superposition is seen in Alice’s description of the final state, though this is not surprising since a SSR violating initial state was assumed. The feature that in Charlie’s description of the final state no coherent superposition of an atom and a molecule is produced in the process is not really surprising, because of the averaging over phase differences in going from Alice’s reference frame to Charlie’s. It is the dependence on the phase $\phi$ imparted during the process that demonstrates coherence (Ramsey interferometry) effects, but it is shown in Appendix 13 that exactly the same results can be obtained via a treatment in which states which are coherent superpositions of an atom and a molecules are never present, the initial BEC state being chosen as a Fock state. In terms of the description by an external observer (Charlie) the claim of violating the super-selection rule has not been demonstrated via this particular process.

2.11.3 Detection of SSR Violating States

Whether such super-selection rule violating states can be detected has also not been justified. For example, consider the state given by a superposition of a one boson state and the vacuum state (as discussed in [72]). We consider an interferometric process in which one mode $A$ for a two mode BEC interferometer is initially in the state $\alpha |0\rangle + \beta |1\rangle$, and the other mode $B$ is initially in the state $|0\rangle$ - thus $|\Psi(i)\rangle = (\alpha |0\rangle + \beta |1\rangle)_A \otimes |0\rangle_B$ in the usual occupancy number notation, where $|\alpha|^2 + |\beta|^2 = 1$. The modes are first coupled by a beam splitter, then a free evolution stage occurs for time $\tau$ associated with a phase difference $\phi = \Delta \tau$ (where $\Delta = \omega_B - \omega_A$ is the mode frequency difference), the modes are then coupled again by the beam splitter and the probability of an atom being found in modes $A$, $B$ finally being measured. The probabilities of finding one atom in modes $A$, $B$ respectively are found to only depend on $|\beta|^2$ and $\phi$. Details are given in Appendix 13. There is no dependence on the relative phase between $\alpha$ and $\beta$, as would be required if the superposition state $\alpha |0\rangle + \beta |1\rangle$ is to be
specified. Exactly the same detection probabilities are obtained if the initial state is the mixed state \( \hat{\rho}(i) = |\alpha|^2 (|0\rangle_A \langle 0| \otimes |0\rangle_B \langle 0|) + |\beta|^2 (|1\rangle_A \langle 1| \otimes |0\rangle_B \langle 0|) \), in which the vacuum state for mode \( A \) occurs with a probability \( |\alpha|^2 \) and the one boson state for mode \( A \) occurs with a probability \( |\beta|^2 \). In this example the proposed coherent superposition associated with the super-selection rule violating state would not be detected in this interferometric process, nor in the more elaborate scheme discussed in [72].

2.12 Super-Selection Rule - Separate Sub-Systems

2.12.1 Local Particle Number SSR

We now consider the role of the super-selection rule for the case of non-entangled states. The global super-selection rule on total particle number has restricted the physical quantum state for a system of identical bosons to be of the form \( \hat{\rho} \). Such states may or may not be entangled states of the modes involved. The question is - do similar restrictions involving the sub-system particle number apply to the modes, considered as separate sub-systems in the definition of non-entangled states? The viewpoint in this paper is that this is so. Note that applying the SSR on the separate sub-system density operators \( \hat{\rho}_X \) is only in the context of non-entangled states. Such a SSR is referred to as a local SSR, as it applies to each of the separate sub-systems. Mathematically, the local particle number SSR can be expressed as

\[
[\hat{N}_X, \hat{\rho}_X^X] = 0
\]

(93)

where \( \hat{N}_X \) is the number operator for sub-system \( X = A, B, \ldots \). The SSR restriction is based on the proposition that the density operators \( \hat{\rho}_A, \hat{\rho}_B, \ldots \) for the separate sub-systems \( A, B, \ldots \) should themselves represent possible physical states for each of the sub-systems, considered as a separate system and thus be required to satisfy the super-selection rule that forbids quantum superpositions of Fock states with differing boson numbers. It is contended that expressions for the non-entangled quantum state \( \hat{\rho} \) in which \( \hat{\rho}_A, \hat{\rho}_B, \hat{\rho}_C, \ldots \) were not physical states for the sub-systems would only be of mathematical interest.

Applying the local particle number SSR to the sub-system density operators for non-entangled states is discussed in papers by Bartlett et al [25, 31] as one of several operational approaches for defining entangled states. However, other authors such as [28, 29] state on the contrary that states when the sub-system density operators do not conform to the local particle number super-selection rule are still separable, others such as [32, 33] do so by implication, so in this paper we are advocating a revision to the widely held notion of entanglement in identical particle systems, the consequence being that the set of entangled states is now much larger. This is a key idea in this paper - not only should super-selection rules on particle numbers be applied to the the overall physical state, entangled or not, but it also should be applied to the density operators that describe states of the modal sub-systems involved in the general definition of non-entangled states. The reasons for adopting this viewpoint are set out
below. Apart from the papers by Bartlett et al \cite{25,31} we are not aware that this definition of non-entangled states has been invoked previously, indeed the opposite approach has been proposed \cite{28,29}. However, the idea of considering whether sub-system states should satisfy the local particle number SSR has been presented in several papers - \cite{28,29,25,31,34,35,36}, mainly in the context of pure states for bosonic systems, though in these papers the focus is on issues other than the definition of entanglement - such as quantum communication protocols \cite{28}, multicopy distillation \cite{25}, mechanical work and accessible entanglement \cite{34,35} and Bell inequality violation \cite{36}. However, there are a number of papers that do not apply the SSR to the sub-system density operators, and those that do have not studied the consequences for various entanglement tests - as is done in the present paper.

\subsection{Local SSR Justification and Independent Local Phase References}

The more elaborate justification in terms of reference frames for this SSR requirement on non-entangled states is presented in SubSection 12.9 of Appendix 12. Essentially the idea is that in the context of separable states, each sub-system has its own independent phase reference frames, and those of Charlie having an unknown phase in relation to those of Alice. This leads to the local particle number SSR.

\subsection{Local SSR Justification and Physics Considerations}

The more simple reasons for this assertion are analogous to those for the overall multi-mode system and may be summarised as: absence of both a preparation process and a measurement process for such states, the lack of need of such states to describe single mode interference and coherence effects. Such superposition states may also be unstable, though again this is not a fatal problem.

Firstly, sub-system states incompatible with the SSR cannot be prepared. Consider for example a typical preparation process. For the situation of two modes \( A, B \) physically allowed pure states \( |\Phi_N\rangle \) could be prepared which in general are entangled states of the form

\[
|\Phi_N\rangle = \sum_{k=0}^{N} A_k^N |k\rangle_A |N-k\rangle_B
\]

so that the general mixed physical state for the two mode system is

\[
\hat{\rho} = \sum_{N=0}^{\infty} \sum_{\Phi} P_{\Phi N} \sum_{k=0}^{N} \sum_{l=0}^{N} A_k^N (A_l^N)^* |k\rangle_A \langle l|_A \otimes |N-k\rangle_B \langle N-l|_B
\]

Hence the reduced density operator - which specifies the state for mode \( A \) if measurements on this mode were carried out and measurements on other modes discarded - will be given by

\[
\hat{\rho}_A = \sum_{N=0}^{\infty} \sum_{\Phi} P_{\Phi N} \sum_{k=0}^{N} A_k^N (A_k^N)^* |k\rangle_A \langle k|_A
\]
which is a statistical mixture of Fock states $|k\rangle_A$. Thus the quantum state for mode $A$ considered separately contains no superposition of states $|k\rangle_A$ with differing numbers of bosons occupying mode $A$. As in the example considered in the previous section, the evolution of $|\Phi_N\rangle$ into a tensor product of superposition states for modes $A$ and $B$ of the form

$$|\Phi_N\rangle = \sum_{k=0}^{N} C_N^k |k\rangle_A \otimes \sum_{k=0}^{N} D_N^k |N-k\rangle_B$$

is not possible. The preparation of the state for mode $A$ must have involved first preparing a physical state for the full multi-mode system - for which the two mode state in Eq. (95) is a specific example - from which the state associated with a particular mode is then determined as given by the reduced density operator. As illustrated by the example just given, the super-selection rule on the total number of identical bosons for the overall system produces a reduced density operator for the sub-system in which the super-selection rule for boson number also applies - that is the state for the sub-system does not involve quantum superpositions of mode Fock states with differing boson numbers, it only can involve statistical mixtures of such states.

Secondly, measurement processes may be applied to each separate mode and again the lack of measurement systems with well defined relativistic phases would preclude measurements that determine the rapidly varying phase differences between the expansion coefficients in single mode state vectors of the form $|\Phi_A\rangle = \sum_{n=0}^{\infty} C_n |n\rangle_A$. Invoking the existence of states whose key properties cannot be measured is somewhat dubious.

Thirdly, experimental setups involving single mode BECs and optical systems can be created and yet there is no need to invoke coherent superpositions of number states to explain coherence and interferometric effects. Thus essentially the same reasons that justify applying the super-selection rule to the overall many boson system also apply to the separate mode sub-systems.

### 2.12.4 Local SSR Justification and Joint Measurements

A consideration of joint measurements on all the sub-systems leads to other fundamental reasons why the individual density operators $\hat{\rho}_A^R, \hat{\rho}_B^R$, in the specific situation of the general mixed non-entangled state given in Eq. (2) must represent physical states for the sub-systems. This state is a statistical mixture of product states $\hat{\rho}_A^R \otimes \hat{\rho}_B^R \otimes \hat{\rho}_C^R \otimes \ldots$ each product state being an overall state of the system that could have been prepared. If sub-sysytem $A$ is prepared by one experimenter in state $\hat{\rho}_A^R$ with probability $P_R$, classical communications to other local experimenters to prepare the other sub-systems in states $\hat{\rho}_B^R, \hat{\rho}_C^R$, etc with the same probability will result in the preparation of the overall mixed state. If such an overall product state is a physical state, then so must be the states of the uncorrelated sub-systems involved. Furthermore, measurements on all the sub-systems can be carried out, not just those on one particular sub-system $A$ - where the results for the sub-system probabilities $P_A(i)$ are determined from
the reduced density operator \( \hat{\rho}_A \) - see Eq. (24). We have seen in Eq (21) that the joint probability \( P_{AB..(i,j..)} \) for measurements on all the sub-systems is determined from the product of the individual sub-system probabilities \( P^R_A(i), P^R_B(j), .. \) associated with sub-system density operators \( \hat{\rho}^A_R, \hat{\rho}^B_R, .. \), the overall product being weighted by the probability \( P_R \) that a particular product state is prepared. The reduced density operators for all the sub-systems do not determine this joint probability - what is required are the full set of sub-system density operators \( \hat{\rho}^A_R, \hat{\rho}^B_R, .. \) along with the overall probability \( P_R \) that a particular product state is prepared. As these individual sub-system probabilities \( P^R_A(i), P^R_B(j), .. \) must determine actual possible measurements then the density operators \( \hat{\rho}^A_R, \hat{\rho}^B_R, .. \) must correspond to possible physical states for the sub-systems, the sub-systems being modes or single particle states in the present case. But as we have seen, the possible physical states that can be prepared for these sub-systems are those as in Eq. (96) which are a statistical mixture of number states with no coherences between Fock states with differing boson numbers, so the \( \hat{\rho}^A_R, \hat{\rho}^B_R, .. \) themselves satisfy the super-selection rule.

### 2.12.5 Example of State that Violate Local and Global Particle Number SSR

Finally, an objection to applying the super-selection rule to separate modes based on emphasising only measurements on only one mode and its the reduced density operator may be raised, and suggest that \( \hat{\rho}^A_R, \hat{\rho}^B_R, .. \) etc may be allowable provided that the overall reduced density operators comply with the super-selection rule. However, as will be seen this is not in general possible. As shown above, measurements on the subsystems with measurements on the other sub-systems discarded - are determined only from the reduced density operators \( \hat{\rho}_A = \sum_R P_R \hat{\rho}^A_R \) alone. Hence it may seem that providing the reduced density operators represent physical states then it does not matter if the \( \hat{\rho}^A_R, \hat{\rho}^B_R, .. \) do not. Indeed, for special cases we can find density operators \( \hat{\rho}^A_R \) that are unphysical even though the contributions \( \hat{\rho}^A_1, \hat{\rho}^A_2 \) are non physical states consisting of pure states that are each quantum superpositions of a zero boson state and a one boson state - in violation of the super-selection rule. However even a minute change in the \( P_R \) will lead to

\[
\hat{\rho}^A_1 = \left( \frac{1}{\sqrt{2}} (|0\rangle_A + |1\rangle_A) \right) \left( \frac{1}{\sqrt{2}} (\langle 0|_A + \langle 1|_A) \right) \quad P_1 = \frac{1}{2}
\]

\[
\hat{\rho}^A_2 = \left( \frac{1}{\sqrt{2}} (|0\rangle_A - |1\rangle_A) \right) \left( \frac{1}{\sqrt{2}} (\langle 0|_A - \langle 1|_A) \right) \quad P_2 = \frac{1}{2}
\]

which yields

\[
\hat{\rho}_A = \frac{1}{2} (|0\rangle_A \langle 0|_A) + \frac{1}{2} (|1\rangle_A \langle 1|_A)
\]
the reduced density operators \( \hat{\rho}_A, \hat{\rho}_B, \ldots \) that are non physical. In the example given, changes to \( P_1 = 0.51 \) and \( P_2 = 0.49 \) will lead to non physical contributions \( |0\rangle_A \langle 1|_A \) and \( |1\rangle_A \langle 0|_A \) to the reduced density operator \( \hat{\rho}_A \). Also, as all the reduced density operators must represent physical states, then the sums in 
\[ \hat{\rho}_A = \sum_R P_R \hat{\rho}_R, \hat{\rho}_B = \sum_R P_R \hat{\rho}_R, \ldots \] must all lead to physical states. Since the probabilities \( P_R \) depend on the preparation process that generates the mixed non-entangled state, and may for example depend on external parameters such as temperature, it would be extremely unlikely for given \( \hat{\rho}_R, \hat{\rho}_B, \ldots \) that all such sums will lead to physical states, though for special choices of the mode density operators and the \( P_R \) this can occur. In addition, the density operators for the other modes must be chosen so that the overall density operator is consistent with the super-selection rule. For example in the case where there are only two modes, the density operators \( \hat{\rho}_B = |0\rangle_B \langle 0|_B \) and \( \hat{\rho}_B = |1\rangle_B \langle 1|_B \) would lead to a physically valid reduced density operator \( \hat{\rho}_B = \frac{1}{2} (|0\rangle_B \langle 0|_B + |1\rangle_B \langle 1|_B) \) for mode \( B \), but there would be terms such as \( \frac{1}{4} |0\rangle_A \langle 1|_A \otimes |0\rangle_B \langle 0|_B \) in the overall density operator, and such a term involves a coherence between an \( N = 0 \) state and an \( N = 1 \) state which is disallowed. Indeed, for the \( \hat{\rho}_A, \hat{\rho}_B \) and \( P_1, P_2 \) as in Eq. (98), there may be no choice for \( \hat{\rho}_B \) and \( \hat{\rho}_B \) that gives rise to an overall physical state. In Appendix 14 the situation where \( \hat{\rho}_B \) and \( \hat{\rho}_B \) are associated with two general pure orthogonal states of the form \( \alpha |0\rangle_B + \beta |1\rangle_B \) and \( -\beta^* |0\rangle_B + \alpha^* |1\rangle_B \) with \( (|\alpha|^2 + |\beta|^2) = 1 \), is considered, and we find that no choice of \( \alpha \) and \( \beta \) leads to an overall physical state - although again the reduced density operator \( \hat{\rho}_B = \frac{1}{2} (|0\rangle_B \langle 0|_B + |1\rangle_B \langle 1|_B) \) is physical.

2.12.6 Example of Global but not Local Particle Number SSR Compliant State

However, in some cases sub-system density operators can be chosen in the context of two mode systems which comply with the global particle number SSR but not the local particle number SSR. Such a case is presented by Verstraete et al [28], [29]. The overall density operator is a statistical mixture

\[ \hat{\rho} = \frac{1}{4} (|\psi_1\rangle \langle \psi_1|)_A \otimes |\psi_1\rangle \langle \psi_1|)_B + \frac{1}{4} (|\psi_i\rangle \langle \psi_i|)_A \otimes |\psi_i\rangle \langle \psi_i|)_B + \frac{1}{4} (|\psi_{-1}\rangle \langle \psi_{-1}|)_A \otimes |\psi_{-1}\rangle \langle \psi_{-1}|)_B + \frac{1}{4} (|\psi_{-i}\rangle \langle \psi_{-i}|)_A \otimes |\psi_{-i}\rangle \langle \psi_{-i}|)_B \]

(100)

where \( |\psi_\omega\rangle = (|0\rangle + \omega |1\rangle)/\sqrt{2} \), with \( \omega = 1, i, -1, -i \). The \( |\psi_\omega\rangle \) are superpositions of zero and one boson states and consequently the local particle number SSR is violated by each of the sub-system density operators \( |\psi_\omega\rangle \langle \psi_\omega|)_A \) and \( |\psi_\omega\rangle \langle \psi_\omega|)_B \). On the other hand, the global particle number SSR is obeyed since the density operator can also be written as

\[ \hat{\rho} = \frac{1}{4} (|0\rangle \langle 0|)_A \otimes |0\rangle \langle 0|)_B + \frac{1}{4} (|1\rangle \langle 1|)_A \otimes |1\rangle \langle 1|)_B + \frac{1}{2} (|\Psi_+\rangle \langle \Psi_+|)_AB \]

(101)
where $|\Psi_+\rangle_{AB} = (|0\rangle_A |1\rangle_B + |1\rangle_A |0\rangle_B)/\sqrt{2}$. This is a statistical mixture of $N = 0, 1, 2$ boson states. Although the expression in Eq. (100) is of the form in Eq. (2), the subsystem density operators $|\psi_\omega\rangle \langle \psi_\omega\rangle_A$ and $|\psi_\omega\rangle \langle \psi_\omega\rangle_B$ do not comply with the local particle number SSR, so this paper the state would be regarded as entangled. However, Verstraete et al \cite{28}, \cite{29} regard it as separable. They would call it separable but nonlocal. However, Eq. (101) indicates that the state could be prepared as a mixed state containing two terms that comply with the local particle number SSR in each of the sub-systems plus a term which is an entangled state of the two sub-systems. The presence of an entangled state in such an obvious preparation process challenges the description of the state as being separable.

2.12.7 General Form of Non-Entangled States

To summarise: basically the sub-systems are single modes that the identical bosons can occupy, the super-selection rule for identical bosons, massive or otherwise, prohibits states which are coherent superpositions of states with different numbers of bosons, and the only physically allowable $\hat{\rho}_A, \hat{\rho}_B, ..$ for the separate mode sub-systems that are themselves compatible with the local particle number SSR are allowed. For single mode sub-systems these can be written as statistical mixtures of states with definite numbers of bosons in the form

$$\hat{\rho}_A = \sum_{n_A} P_{n_A} |n_A\rangle \langle n_A|, \quad \hat{\rho}_B = \sum_{n_B} P_{n_B} |n_B\rangle \langle n_B| \ldots (102)$$

However, in cases where the sub-systems are pairs of modes the density operators $\hat{\rho}_A, \hat{\rho}_B, ..$ for the separate sub-systems are still required to conform to the symmetrisation principle and the super-selection rule. The forms for $\hat{\rho}_A, \hat{\rho}_B, ..$ are now of course more complex, as entanglement within the pairs of modes $A_1, A_2$ associated with sub-system $A$, the pairs of modes $B_1, B_2$ associated with sub-system $B$, etc is now possible within the definition for the general non-entangled state Eq. (2) for these pairs of modes. Within each pair of modes $A_1, A_2$ statistical mixtures of states with differing total numbers $N_A$ bosons in the two modes are possible and the sub-system density operators are based on states of the form given in Eq. (85). We have

$$|\Phi_{N_A}\rangle_A = \sum_{k=0}^{N_A} C_A \phi(N_A, k) |k\rangle_{A_1} \otimes |N_A - k\rangle_{A_2}$$

$$\hat{\rho}_A = \sum_{N_A=0}^{\infty} \sum_{\Phi} P_{\Phi N_A} |\Phi_{N_A}\rangle_A \langle \Phi_{N_A}|_A \ldots (103)$$

with analogous expressions for the density operators $\hat{\rho}_B$ etc for the other pairs of modes. Note that $|\Phi_{N_A}\rangle_A$ only involves quantum superpositions of states with the same total number of bosons $N_A$. The expression (213) in SubSection 5.3 is of this form.
2.13 Two Mode Coherent State Mixture

To further illustrate some of the points made about super-selection rules - local and global - it is useful to consider a specific case also presented by Verstraete et al [28], [29]. This mixture of two mode coherent states is represented by the two mode density operator

\[ \hat{\rho} = \int \frac{d\theta}{2\pi} |\alpha,\alpha\rangle \langle \alpha,\alpha| \]
\[ = \int \frac{d\theta}{2\pi} (|\alpha\rangle \langle \alpha|)_A \otimes (|\alpha\rangle \langle \alpha|)_B \]  

(104)

where $|\alpha\rangle_C$ is a one mode coherent state for mode $C = A, B$ with $\alpha = |\alpha| \exp(-i\theta)$, and modes $A, B$ are associated with bosonic annihilation operators $\hat{a}, \hat{b}$. The magnitude $|\alpha|$ is fixed.

This density operator appears to be that for a non-entangled state of modes $A, B$ in the form

\[ \hat{\rho} = \sum_R P_R \hat{\rho}^A_R \otimes \hat{\rho}^B_R \]  

(105)

with $\sum_R P_R \to \int \frac{d\theta}{2\pi}$ and $\hat{\rho}^A_R \to (|\alpha\rangle \langle \alpha|)_A$ and $\hat{\rho}^B_R \to (|\alpha\rangle \langle \alpha|)_B$. However although this choice of $\hat{\rho}^A_R, \hat{\rho}^B_R$ satisfy the Hermitiancy, unit trace, positivity features they do not conform to the requirement of satisfying the (local) sub-system boson number super-selection rule. From Eq. (104) we have

\[ \langle n | (|\alpha\rangle \langle \alpha|) | m \rangle_A = \exp(-|\alpha|^2) \frac{\alpha^n}{\sqrt{n!}} \frac{\alpha^m}{\sqrt{m!}} \]
\[ \langle p | (|\alpha\rangle \langle \alpha|) | q \rangle_B = \exp(-|\alpha|^2) \frac{\alpha^p}{\sqrt{p!}} \frac{\alpha^q}{\sqrt{q!}} \]  

(106)

so clearly for each of the separate modes there are coherences between Fock states with differing boson occupation numbers. In the approach in the present paper the density operator in Eq. (104) does not represent a non-entangled state. However, in the papers of Verstraete et al [28], [29], Hillery et al [32], [33] and others it would represent an allowable non-entangled (separable) state. Indeed, Verstraete et al [28] specifically state ". this state is obviously separable, though the states $|\alpha\rangle$ are incompatible with the (local) super-selection rule.". Verstraete et al [28] introduce the state defined in Eq. (104) as an example of a state that is separable (in their terms) but which cannot be prepared locally, because it is incompatible with the local particle number super-selection rule.

The mixture of two mode coherent states does of course satisfy the total or global boson number super-selection rule. The matrix elements between two mode Fock states are

\[ \langle n | (|\alpha\rangle \langle \alpha|) | m \rangle_A \otimes \langle p | (|\alpha\rangle \langle \alpha|) | q \rangle_B \]  

\[ = \exp(-2|\alpha|^2) \frac{|\alpha|^{n+m}}{\sqrt{n!} \sqrt{m!}} \frac{|\alpha|^{p+q}}{\sqrt{p!} \sqrt{q!}} \int \frac{d\theta}{2\pi} \exp(-i(n - m + p - q)\theta) \]
\[ = \exp(-2|\alpha|^2) \frac{|\alpha|^{n+m}}{\sqrt{n!} \sqrt{m!}} \frac{|\alpha|^{p+q}}{\sqrt{p!} \sqrt{q!}} \delta_{n+m,p+q} \]  

(107)
These overall matrix elements are zero unless \( n + p = m + q \), showing that there are no coherences between two mode Fock states where the total boson number differs. The mixture of two mode coherent states has the interesting feature of providing an example of a two mode state which satisfies the global but not the local super-selection rule.

The reduced density operators for modes \( A, B \) are

\[
\hat{\rho}_{A} = \int \frac{d\theta}{2\pi} (|\alpha\rangle \langle \alpha|)_{A} \quad \hat{\rho}_{B} = \int \frac{d\theta}{2\pi} (|\alpha\rangle \langle \alpha|)_{B}
\]

and a straightforward calculation gives

\[
\hat{\rho}_{A} = \exp(-|\alpha|^{2}) \sum_{n} \frac{|\alpha|^{2n}}{n!} (|n\rangle \langle n|)_{A} \quad \hat{\rho}_{B} = \exp(-|\alpha|^{2}) \sum_{p} \frac{|\alpha|^{2p}}{p!} (|p\rangle \langle p|)_{B}
\]

which are statistical mixtures of Fock states with the expected Poisson distribution associated with coherent states. This shows that the reduced density operators are consistent with the separate mode local super-selection rule, whereas the density operators \( \hat{\rho}_{A} = (|\alpha\rangle \langle \alpha|)_{A} \), \( \hat{\rho}_{B} = (|\alpha\rangle \langle \alpha|)_{B} \) are not. Later we will revisit this example in the context of entanglement tests.

Note that if a twirling operation (see Eq. (315)) were to be applied to mode \( A \), the result would be equivalent to applying two independent twirling operations to each mode. In this case the density operator for each mode is a Poisson statistical mixture of number states, so each mode has a density operator that complies with the local particle number SSR.

### 2.14 Two Mode System - Coherence Terms

The general non-entangled state for modes \( \hat{a} \) and \( \hat{b} \) is given by

\[
\hat{\rho} = \sum_{R} P_{R} \hat{\rho}_{A}^{R} \otimes \hat{\rho}_{B}^{R}
\]

and as a consequence of the requirement that \( \hat{\rho}_{A}^{R} \) and \( \hat{\rho}_{B}^{R} \) are physical states for modes \( \hat{a} \) and \( \hat{b} \) satisfying the super-selection rule, it follows that

\[
\langle (\hat{a})^{n} \rangle_{a} = Tr(\hat{\rho}_{A}^{R}(\hat{a})^{n}) = 0 \quad \langle (\hat{b})^{m} \rangle_{b} = Tr(\hat{\rho}_{B}^{R}(\hat{b})^{m}) = 0
\]

Thus coherence terms are zero. As we will see these results will limit spin squeezing to entangled states of modes \( \hat{a} \) and \( \hat{b} \). Note that similar results also apply when non-entangled states for the original modes \( \hat{c} \) and \( \hat{d} \) are considered - \( \langle (\hat{c})^{n} \rangle_{c} = 0 \), etc..
2.15 Two Sub-Systems of Pairs of Modes - Coherence Terms

In this case the general non-entangled state where $A$ and $B$ are pairs of modes - $A_1, A_2$ associated with sub-system $A$, and modes $B_1, B_2$ associated with sub-system $B$, the overall density operator is of the form (130), with $C \rightarrow A$, $D \rightarrow B$, whilst the sub-system density operators are of the forms given in (103). In this case we now have in general

$$
\langle (\hat{a}_i)^n \rangle_A = Tr(\hat{\rho}_R^A(\hat{a}_i)^n) \neq 0 \quad \langle (\hat{a}_i^\dagger)^n \rangle_A = Tr(\hat{\rho}_R^A(\hat{a}_i^\dagger)^n) \neq 0
$$

$$
\langle (\hat{b}_j)^m \rangle_B = Tr(\hat{\rho}_R^B(\hat{b}_j)^m) \neq 0 \quad \langle (\hat{b}_j^\dagger)^m \rangle_B = Tr(\hat{\rho}_R^B(\hat{b}_j^\dagger)^m) \neq 0
$$

$$
i, j = 1, 2 \quad (110)
$$

so unlike the case where the two sub-systems are single modes, there are non-zero coherences when they are pairs of modes.
3 Spin Squeezing

The basic concept of spin squeezing was first introduced by Kitagawa and Ueda [44] for general spin systems. These include cases based on two mode systems, such as may occur both for optical fields and for Bose-Einstein condensates. Though focused on systems of massive identical bosons, the treatment in this paper also applies to photons though details will differ.

3.1 Spin Operators, Bloch Vector and Covariance Matrix

3.1.1 Spin Operators

For two mode systems with mode annihilation operators $\hat{a}, \hat{b}$ associated with the two single particle states $|\phi_a\rangle, |\phi_b\rangle$, and where the non-zero bosonic commutation rules are $[\hat{c}, \hat{c}^\dagger] = 1$ ($\hat{c} = \hat{a}$ or $\hat{b}$), Schwinger spin angular momentum operators $\hat{S}_\xi$ ($\xi = x, y, z$) are defined as

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

and which satisfy the commutation rules $[\hat{S}_\xi, \hat{S}_\mu] = i\epsilon_{\xi\mu\lambda} \hat{S}_\lambda$ for angular momentum operators. For bosons the square of the angular momentum operators is given by $\hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 = (N/2)(N/2 + 1)$, where $N = (\hat{b}^\dagger \hat{b} + \hat{a}^\dagger \hat{a})$ is the boson total number operator, those for the separate modes being $\hat{n}_c = \hat{c}^\dagger \hat{c}$ ($\hat{c} = \hat{a}$ or $\hat{b}$). The Schwinger spin operators are the second quantization form of symmetrized one body operators $\hat{S}_x = \sum_i (|\phi_b(i)\rangle \langle \phi_a(i)| + |\phi_a(i)\rangle \langle \phi_b(i)|)/2$ ; $\hat{S}_y = \sum_i (|\phi_b(i)\rangle \langle \phi_a(i)| - |\phi_a(i)\rangle \langle \phi_b(i)|)/2i$ ; $\hat{S}_z = \sum_i (|\phi_b(i)\rangle \langle \phi_a(i)| - |\phi_a(i)\rangle \langle \phi_b(i)|)/2$, where the sum $i$ is over the identical bosonic particles. In the case of the two mode EM field the spin angular momentum operators are related to the Stokes parameters.

3.1.2 Bloch Vector and Covariance Matrix

If the density operator for the overall system is $\hat{\rho}$ then expectation values of the three spin operators $\langle \hat{S}_\xi \rangle = Tr(\hat{\rho} \hat{S}_\xi)$ ($\xi = x, y, z$) define the Bloch vector. Spin squeezing is related to the fluctuation operators $\Delta \hat{S}_\xi = \hat{S}_\xi - \langle \hat{S}_\xi \rangle$, in terms of which a real, symmetric covariance matrix $C(\hat{S}_\xi, \hat{S}_\mu)$ ($\xi, \mu = x, y, z$) is defined [72], [65] via

$$C(\hat{S}_\xi, \hat{S}_\mu) = \left( \langle \Delta \hat{S}_\xi \Delta \hat{S}_\mu \rangle + \langle \Delta \hat{S}_\mu \Delta \hat{S}_\xi \rangle \right)/2$$

$$= \langle \hat{S}_\xi \hat{S}_\mu + \hat{S}_\mu \hat{S}_\xi \rangle/2 - \langle \hat{S}_\xi \rangle \langle \hat{S}_\mu \rangle$$

and whose diagonal elements $C(\hat{S}_\xi, \hat{S}_\xi) = \langle \Delta \hat{S}_\xi^2 \rangle$ gives the variance for the fluctuation operators. The variances for the spin operators satisfy the three Heisenberg uncertainty principle relations $\langle \Delta \hat{S}_x^2 \rangle \langle \Delta \hat{S}_y^2 \rangle \geq \frac{1}{4} \langle \Delta \hat{S}_z \rangle^2$ ; $\langle \Delta \hat{S}_x^2 \rangle \langle \Delta \hat{S}_z^2 \rangle \geq \frac{1}{4} \langle \Delta \hat{S}_y \rangle^2$ ; $\langle \Delta \hat{S}_y^2 \rangle \langle \Delta \hat{S}_z^2 \rangle \geq \frac{1}{4} \langle \Delta \hat{S}_x \rangle^2$.
\[ \frac{1}{4} |\langle \hat{S}_x \rangle|^2; \langle \Delta \hat{S}_x^2 \rangle \langle \Delta \hat{S}_x^2 \rangle \geq \frac{1}{4} |\langle \hat{S}_y \rangle|^2, \]  
and spin squeezing is usually defined via conditions such as  
\[ \langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_y \rangle| \text{ with } \langle \Delta \hat{S}_y^2 \rangle > \frac{1}{2} |\langle \hat{S}_z \rangle|, \]  
for \( \hat{S}_x \) being squeezed compared to \( \hat{S}_y \) and so on. However this definition is unsatisfactory since it ignores the presence of the off-diagonal elements of the covariance matrix, so a better definition is required.

### 3.2 New Spin Operators and Principal Spin Fluctuations

The covariance matrix has real, non-negative eigenvalues and can be diagonalised via an orthogonal rotation matrix \( M(-\alpha, -\beta, -\gamma) \) that defines new spin angular momentum operators \( \hat{J}_\xi (\xi = x, y, z) \) via

\[
\hat{J}_\xi = \sum_\mu M_{\xi\mu}(-\alpha, -\beta, -\gamma) \hat{S}_\mu \quad (113)
\]

and where

\[
C(\hat{J}_\xi, \hat{J}_\mu) = \sum_{\lambda\theta} M_{\xi\lambda}(-\alpha, -\beta, -\gamma) C(\hat{S}_\lambda, \hat{S}_\theta) M_{\mu\theta}(-\alpha, -\beta, -\gamma) = \delta_{\xi\mu} \langle \Delta \hat{J}_\xi^2 \rangle \quad (114)
\]

is the covariance matrix for the new spin angular momentum operators \( \hat{J}_\xi (\xi = x, y, z) \), and which is diagonal with the diagonal elements \( \langle \Delta \hat{J}_x^2 \rangle \), \( \langle \Delta \hat{J}_y^2 \rangle \) and \( \langle \Delta \hat{J}_z^2 \rangle \) giving the so-called principal spin fluctuations. The matrix \( M(\alpha, \beta, \gamma) \) is parameterised in terms of three Euler angles \( \alpha, \beta, \gamma \) and is given in [74] (see Eq. (4.43)).

The Bloch vector and spin fluctuations are illustrated in Figure 1. In Fig 1 the Bloch vector and spin fluctuation ellipsoid is shown in terms of the original spin operators \( \hat{S}_\xi (\xi = x, y, z) \)

Figure 1 near here.

### 3.3 Spin Squeezing for New Spin Operators

#### 3.3.1 Heisenberg Uncertainty Principle and Spin Squeezing

Since the new spin operators also satisfy Heisenberg uncertainty principle relationships

\[
\begin{align*}
\langle \Delta \hat{J}_x^2 \rangle \langle \Delta \hat{J}_y^2 \rangle & \geq \frac{1}{4} |\langle \hat{J}_z \rangle|^2 \\
\langle \Delta \hat{J}_y^2 \rangle \langle \Delta \hat{J}_z^2 \rangle & \geq \frac{1}{4} |\langle \hat{J}_x \rangle|^2 \\
\langle \Delta \hat{J}_z^2 \rangle \langle \Delta \hat{J}_x^2 \rangle & \geq \frac{1}{4} |\langle \hat{J}_y \rangle|^2
\end{align*}
\quad (115)
\]

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spin squeezing will now be defined via conditions such as

\[
\langle \Delta \hat{J}_x^2 \rangle < \frac{1}{2} \langle \hat{J}_x \rangle \quad \text{and} \quad \langle \Delta \hat{J}_y^2 \rangle > \frac{1}{2} \langle \hat{J}_x \rangle \\
\langle \Delta \hat{J}_y^2 \rangle < \frac{1}{2} \langle \hat{J}_y \rangle \quad \text{and} \quad \langle \Delta \hat{J}_x^2 \rangle > \frac{1}{2} \langle \hat{J}_x \rangle \\
\langle \Delta \hat{J}_z^2 \rangle < \frac{1}{2} \langle \hat{J}_y \rangle \quad \text{and} \quad \langle \Delta \hat{J}_x^2 \rangle > \frac{1}{2} \langle \hat{J}_y \rangle 
\]

for \( \hat{J}_y \) being squeezed compared to \( \hat{J}_x \), and so on. By convention we may choose \( \langle \Delta \hat{J}_x^2 \rangle \leq \langle \Delta \hat{J}_y^2 \rangle \leq \langle \Delta \hat{J}_z^2 \rangle \), so the primary spin operator of interest will be \( \hat{J}_x \) since this has the smallest fluctuation. Note that here we have chosen principal spin fluctuations, but of course the last Heisenberg uncertainty relations apply for any new choice of rotated spin operators - as occurs in the next part of this section.

3.3.2 Alternative Spin Squeezing Criteria

Other criteria for spin squeezing are also used, for example in the article by Wineland et al [75]. To focus on spin squeezing for \( \hat{J}_x \) compared to any orthogonal spin operators we can combine the first and third Heisenberg uncertainty principle relationships to give

\[
\langle \Delta \hat{J}_x^2 \rangle \left( \langle \Delta \hat{J}_y^2 \rangle + \langle \Delta \hat{J}_z^2 \rangle \right) \geq \frac{1}{4} \left( \langle \hat{J}_y \rangle^2 + \langle \hat{J}_z \rangle^2 \right) \tag{116}
\]

Then we may define two new spin operators via

\[
\hat{J}_{\perp 1} = \cos \theta \, \hat{J}_y + \sin \theta \, \hat{J}_z \quad \hat{J}_{\perp 2} = -\sin \theta \, \hat{J}_y + \cos \theta \, \hat{J}_z \tag{118}
\]

where \( \theta \) corresponds to a rotation angle in the \( yz \) plane, and which satisfy the standard angular momentum commutation rules \([\hat{J}_{\perp 1}, \hat{J}_{\perp 2}] = i \hat{J}_x, [\hat{J}_{\perp 2}, \hat{J}_{\perp 1}] = i \hat{J}_y, [\hat{J}_{\perp 1}, \hat{J}_y] = i \hat{J}_{\perp 2} \). It is straightforward to show that \( \langle \Delta \hat{J}_{\perp 1}^2 \rangle + \langle \Delta \hat{J}_{\perp 2}^2 \rangle = \langle \Delta \hat{J}_x^2 \rangle \) and \( \langle \hat{J}_{\perp 1} \rangle^2 + \langle \hat{J}_{\perp 2} \rangle^2 = \langle \hat{J}_y \rangle^2 + \langle \hat{J}_z \rangle^2 \) so that

\[
\langle \Delta \hat{J}_{\perp 1}^2 \rangle \left( \langle \Delta \hat{J}_{\perp 2}^2 \rangle + \langle \Delta \hat{J}_{\perp 2}^2 \rangle \right) \geq \frac{1}{4} \left( \langle \hat{J}_{\perp 1} \rangle^2 + \langle \hat{J}_{\perp 2} \rangle^2 \right) \tag{119}
\]

so that spin squeezing for \( \hat{J}_x \) compared to any two orthogonal spin operators such as \( \hat{J}_{\perp 1} \) or \( \hat{J}_{\perp 2} \) would be defined as

\[
\langle \Delta \hat{J}_{\perp 1}^2 \rangle < \frac{1}{2} \sqrt{\langle \hat{J}_{\perp 1} \rangle^2 + \langle \hat{J}_{\perp 2} \rangle^2} \quad \text{and} \quad \langle \Delta \hat{J}_{\perp 1}^2 \rangle + \langle \Delta \hat{J}_{\perp 2}^2 \rangle > \frac{1}{2} \sqrt{\langle \hat{J}_{\perp 1} \rangle^2 + \langle \hat{J}_{\perp 2} \rangle^2} \tag{120}
\]
This criterion would apply however the choice of rotation matrix $M(-\alpha, -\beta, -\gamma)$ is made, so $\Delta \hat{J}_x$ does not have to correspond to the principal spin fluctuation with the smallest variance though obviously such a choice is preferable over some arbitrary set of new spin operators. For spin squeezing in $\langle \Delta \hat{J}_x^2 \rangle$ we require

$$\xi^2 = \frac{\langle \Delta \hat{J}_x^2 \rangle}{\left( |\langle \hat{J}_{\perp 1} \rangle|^2 + |\langle \hat{J}_{\perp 2} \rangle|^2 \right)} < \frac{1}{2} \sqrt{\frac{1}{|\langle \hat{J}_{\perp 1} \rangle|^2 + |\langle \hat{J}_{\perp 2} \rangle|^2}} \sim \frac{1}{N} \quad (121)$$

The last step is an approximation based on the assumption that the Bloch vector lies in the $yz$ plane and close to the Bloch sphere, this situation being the most conducive to detecting the fluctuation $\langle \Delta \hat{J}_x^2 \rangle$. In this situation $\sqrt{\left( |\langle \hat{J}_{\perp 1} \rangle|^2 + |\langle \hat{J}_{\perp 2} \rangle|^2 \right)}$ is approximately $N/2$. The condition $\xi^2 < 1/N$ is sometimes taken as the condition for spin squeezing [76], but it should be noted that this is approximate and Eq. (120) gives the correct expression.

### 3.3.3 Planar Spin Squeezing

A special case of recent interest is that referred to as planar squeezing [77] in which the Bloch vector for a suitable choice of spin operators lies in a plane and along one of the axes. If this plane is chosen to be the $xy$ plane and the $x$ axis is chosen then $\langle \hat{J}_z \rangle = 0$ and $\langle \hat{J}_y \rangle = 0$, resulting in only one Heisenberg uncertainty principle relationship where the right side is non-zero, namely $\langle \Delta \hat{J}_y^2 \rangle \langle \Delta \hat{J}_x^2 \rangle \gtrsim \frac{1}{2} |\langle \hat{J}_x \rangle|^2$. Combining this with $\langle \Delta \hat{J}_y^2 \rangle \langle \Delta \hat{J}_x^2 \rangle \geq 0$ gives

$$\langle \Delta \hat{J}_y^2 \rangle \langle \Delta \hat{J}_x^2 \rangle \gtrsim \frac{1}{2} |\langle \hat{J}_x \rangle|^2.$$  So the total spin fluctuation in the $xy$ plane defined as $\langle \Delta \hat{J}_\parallel^2 \rangle = \langle \Delta \hat{J}_y^2 \rangle + \langle \Delta \hat{J}_x^2 \rangle$ will be squeezed compared to the total spin fluctuation perpendicular to the $xy$ plane given by $\langle \Delta \hat{J}_\perp^2 \rangle = \langle \Delta \hat{J}_z^2 \rangle$ if

$$\langle \Delta \hat{J}_\parallel^2 \rangle < \frac{1}{2} |\langle \hat{J}_x \rangle| \quad \text{and} \quad \langle \Delta \hat{J}_\perp^2 \rangle > \frac{1}{2} |\langle \hat{J}_x \rangle| \quad (122)$$

By minimising $\langle \Delta \hat{J}_\parallel^2 \rangle$ whilst satisfying the constraints $\langle \hat{J}_y \rangle = 0$ a spin squeezed state is found that satisfies (122) with $\langle \Delta \hat{J}_y^2 \rangle \sim J^{2/3}$, $\langle \Delta \hat{J}_x^2 \rangle \sim J^{4/3}$, $\langle \hat{J}_y \rangle \sim J$ for large $J = N/2$ [77]. The Bloch vector is on the Bloch sphere and condition (121) is also satisfied.
3.4 Rotation Operators and New Modes

3.4.1 Rotation Operators

The new spin operators are also related to the original spin operators via a unitary rotation operator $\hat{R}(\alpha, \beta, \gamma)$ parameterised in terms of Euler angles so that

$$\hat{J}_\xi = \hat{R}(\alpha, \beta, \gamma) \hat{S}_\xi \hat{R}(\alpha, \beta, \gamma)^{-1}$$  \hspace{1cm} (123)

where

$$\hat{R}(\alpha, \beta, \gamma) = \hat{R}_z(\alpha) \hat{R}_y(\beta) \hat{R}_z(\gamma)$$  \hspace{1cm} (124)

with $\hat{R}_\xi(\phi) = \exp(i\phi \hat{S}_\xi)$ describing a rotation about the $\xi$ axis anticlockwise through an angle $\phi$. Details for the rotation operators and matrices are set out in [65]. Note that Eq. (123) specifies a rotation of the vector spin operator rather than a rotation of the axes, so $\hat{J}_\xi$ ($\xi = x, y, z$) are the components of the rotated vector spin operator with respect to the original axes.

3.4.2 New Mode Operators

We can also see that the new spin operators are related to new mode operators $\hat{c}$ and $\hat{d}$ via

$$\hat{J}_x = (\hat{d}^\dagger \hat{c} + \hat{c}^\dagger \hat{d})/2 \hspace{1cm} \hat{J}_y = (\hat{d}^\dagger \hat{c} - \hat{c}^\dagger \hat{d})/2i \hspace{1cm} \hat{J}_z = (\hat{d}^\dagger \hat{d} - \hat{c}^\dagger \hat{c})/2$$  \hspace{1cm} (125)

where

$$\hat{c} = \hat{R}(\alpha, \beta, \gamma) \hat{a} \hat{R}(\alpha, \beta, \gamma)^{-1} \hspace{1cm} \hat{d} = \hat{R}(\alpha, \beta, \gamma) \hat{b} \hat{R}(\alpha, \beta, \gamma)^{-1}$$  \hspace{1cm} (126)

For the bosonic case a straight-forward calculation gives the new mode operators as

$$\hat{c} = \exp\left(\frac{i}{2} \gamma\right) \left( \cos\left(\frac{\beta}{2}\right) \exp\left(\frac{i}{2} \alpha\right) \hat{a} + \sin\left(\frac{\beta}{2}\right) \exp\left(-\frac{i}{2} \alpha\right) \hat{b} \right)$$

$$\hat{d} = \exp\left(-\frac{i}{2} \gamma\right) \left( -\sin\left(\frac{\beta}{2}\right) \exp\left(\frac{i}{2} \alpha\right) \hat{a} + \cos\left(\frac{\beta}{2}\right) \exp\left(-\frac{i}{2} \alpha\right) \hat{b} \right)$$

and it is easy to then check that $\hat{c}$ and $\hat{d}$ satisfy the expected non-zero bosonic commutation rules are $[\hat{c}, \hat{c}^\dagger] = 1$ ($\hat{c} = \hat{c}$ or $\hat{d}$) and that the total boson number operator is $\hat{N} = (\hat{d}^\dagger \hat{d} + \hat{c}^\dagger \hat{c})$. As $\hat{N}$ is invariant under unitary rotation operators it follows that $\hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 = (\hat{N}/2)(\hat{N}/2 + 1)$. 

60
3.4.3 New Modes

The new mode operators correspond to new single particle states $|\phi_c\rangle$, $|\phi_d\rangle$ where

$$
|\phi_c\rangle = \exp(-\frac{1}{2}i\gamma) \left( \cos(\frac{\beta}{2}) \exp(-\frac{1}{2}i\alpha) |\phi_a\rangle + \sin(\frac{\beta}{2}) \exp(\frac{1}{2}i\alpha) |\phi_b\rangle \right)
$$

$$
|\phi_d\rangle = \exp(\frac{1}{2}i\gamma) \left( -\sin(\frac{\beta}{2}) \exp(-\frac{1}{2}i\alpha) |\phi_a\rangle + \cos(\frac{\beta}{2}) \exp(\frac{1}{2}i\alpha) |\phi_b\rangle \right)
$$

These are two orthonormal quantum superpositions of the original single particle states $|\phi_a\rangle$, $|\phi_b\rangle$, and as such represent an alternative choice of modes that could be realised experimentally.

Eqs. (127) can be inverted to give the old mode operators via

$$
\hat{a} = \exp(-\frac{1}{2}i\alpha) \left( \cos(\frac{\beta}{2}) \exp(\frac{1}{2}i\gamma) \hat{c} - \sin(\frac{\beta}{2}) \exp(\frac{1}{2}i\gamma) \hat{d} \right)
$$

$$
\hat{b} = \exp(+\frac{1}{2}i\alpha) \left( \sin(\frac{\beta}{2}) \exp(\frac{1}{2}i\gamma) \hat{c} + \cos(\frac{\beta}{2}) \exp(-\frac{1}{2}i\gamma) \hat{d} \right)
$$

(129)

3.5 Two Mode System - Coherence Terms

For our two-mode case we have also seen that the original choice of modes with annihilation operators $\hat{a}$ and $\hat{b}$ may be replaced by new modes with annihilation operators $\hat{c}$ and $\hat{d}$. Since the new modes are associated with new spin operators $\hat{J}_\xi (\xi = x, y, z)$ for which the covariance matrix is diagonal and where the diagonal elements give the variances that are relevant for the definition of spin squeezing, it is therefore more relevant to consider entanglement for the case where the sub-systems are modes $\hat{c}$ and $\hat{d}$, rather than $\hat{a}$ and $\hat{b}$. Consequently the general non-entangled state for modes $\hat{c}$ and $\hat{d}$ is given by

$$
\hat{\rho} = \sum_R P_R \hat{\rho}_R^C \otimes \hat{\rho}_R^D
$$

(130)

and as a consequence of the requirement that $\hat{\rho}_R^C$ and $\hat{\rho}_R^D$ are physical states for modes $\hat{c}$ and $\hat{d}$ satisfying the super-selection rule, it follows that

$$
\langle \hat{c}^n \rangle_c = \text{Tr}(\hat{\rho}_R^C (\hat{c}^n)) = 0 \quad \langle \hat{c}^\dagger^n \rangle_c = \text{Tr}(\hat{\rho}_R^C (\hat{c}^\dagger)^n) = 0
$$

$$
\langle \hat{d}^m \rangle_d = \text{Tr}(\hat{\rho}_R^D (\hat{d}^m)) = 0 \quad \langle \hat{d}^\dagger^m \rangle_d = \text{Tr}(\hat{\rho}_R^D (\hat{d}^\dagger)^m) = 0
$$

(131)

Thus coherence terms are zero. As we will see these results will limit spin squeezing to entangled states of modes $\hat{c}$ and $\hat{d}$.
3.6 Quantum Correlation Functions and Measurements

Finally, we note that the principal spin fluctuations can be related to quantum correlation functions. For example, it is easy to show that

$$\langle \Delta \hat{J}_x^2 \rangle = \frac{1}{4} \left( \langle (\hat{d}^\dagger)^2 (\hat{c})^2 \rangle + \langle (\hat{c}^\dagger)^2 (\hat{d})^2 \rangle + 2 \langle \hat{d}^\dagger \hat{c}^\dagger \hat{c} \hat{d} \rangle + \langle \hat{c}^\dagger \hat{c} \rangle \right)$$

$$- \frac{1}{4} \left( \langle (\hat{d}^\dagger \hat{c})^2 \rangle + \langle (\hat{c}^\dagger \hat{d})^2 \rangle + 2 \langle \hat{d}^\dagger \hat{c} \rangle \langle \hat{c} \hat{d} \rangle \right)$$

showing that $$\langle \Delta \hat{J}_x^2 \rangle$$ is related to various first and second order quantum correlation functions. These can be measured experimentally and are given theoretically in terms of phase space integrals involving distribution functions to represent the density operator and phase space variables to represent the mode annihilation, creation operators.
4 Spin Squeezing as a Test for Entanglement

With the general non-entangled state now required to be such that the density operators for the individual sub-systems must represent physical states and conform to the super-selection rule, the consequential link between entanglement in two mode bosonic systems and spin squeezing can now be established. We first consider spin squeezing for the principal spin operators \( \hat{J}_x \), \( \hat{J}_y \), \( \hat{J}_z \) and entangled states of the related new modes \( \hat{c}, \hat{d} \) and then spin squeezing for the original spin operators \( \hat{S}_x \), \( \hat{S}_y \), \( \hat{S}_z \) and entangled states of the original modes \( \hat{a}, \hat{b} \). Examples of entangled states that are not spin squeezed and states that are not entangled nor spin squeezed for one choice of mode sub-systems, but are entangled and spin squeezed for another choice are then presented.

4.1 Spin Squeezing Requires Entanglement

Firstly, the variance for a Hermitian operator \( \hat{\Omega} \) in a mixed state \( \hat{\rho} = \sum_R P_R \hat{\rho}_R \) (133) is always greater than or equal to the the average of the variances for the separate components

\[
\left< \Delta \hat{\Omega}^2 \right> \geq \sum_R P_R \left< \Delta \hat{\Omega}_R^2 \right>
\]

(134)

where \( \left< \Delta \hat{\Omega}^2 \right> = Tr(\hat{\rho} \Delta \hat{\Omega}^2) \) with \( \Delta \hat{\Omega} = \hat{\Omega} - \left< \hat{\Omega} \right> \) and \( \left< \Delta \hat{\Omega}_R^2 \right> = Tr(\hat{\rho}_R \Delta \hat{\Omega}_R^2) \) with \( \Delta \hat{\Omega}_R = \hat{\Omega} - \left< \hat{\Omega} \right>_R \). The proof is straightforward and given in Ref. [78].

4.1.1 Cases of \( \hat{J}_x \) and \( \hat{J}_y \)

Next we calculate \( \left< \Delta \hat{J}_x^2 \right>_R \), \( \left< \Delta \hat{J}_y^2 \right>_R \) and \( \left< \hat{J}_x \right>_R \), \( \left< \hat{J}_y \right>_R \), \( \left< \hat{J}_z \right>_R \) for the case where \( \hat{\rho}_R = \hat{\rho}_R \otimes \hat{\rho}_R \). From Eqs. (125) we find that

\[
\hat{J}_x^2 = \frac{1}{4}((\hat{d}^\dagger)^2(\hat{c})^2 + \hat{d}\hat{d}^\dagger \hat{c}\hat{c} + \hat{c}\hat{d}^\dagger \hat{d}\hat{c} + (\hat{d})^2(\hat{c})^2)
\]

(135)

so that on taking the trace with \( \hat{\rho} \) and using Eqs. (131) we get after applying the commutation rules \([\hat{c}, \hat{c}^\dagger] = \hat{1} \) (\( \hat{c} = \hat{c} \) or \( \hat{d} \))

\[
\begin{align*}
\left< \hat{J}_x \right>_R & = \frac{1}{4}(\left< \hat{d}\hat{d}^\dagger \right>_R + \left< \hat{c}\hat{c}^\dagger \right>_R) + \frac{1}{2}(\left< \hat{c}\hat{c}^\dagger \right>_R \left< \hat{d}\hat{d}^\dagger \right>_R) \\
\left< \hat{J}_y \right>_R & = \frac{1}{4}(\left< \hat{d}\hat{d}^\dagger \right>_R + \left< \hat{c}\hat{c}^\dagger \right>_R) + \frac{1}{2}(\left< \hat{c}\hat{c}^\dagger \right>_R \left< \hat{d}\hat{d}^\dagger \right>_R)
\end{align*}
\]

(136)
As we also have

\[ \langle \hat{J}_x \rangle_R = \frac{1}{2}(\langle \hat{d}^\dagger \rangle_R \langle \hat{c} \rangle_R + \langle \hat{c}^\dagger \rangle_R \langle \hat{d} \rangle_R) = 0 \]

\[ \langle \hat{J}_y \rangle_R = \frac{1}{2i}(\langle \hat{d}^\dagger \rangle_R \langle \hat{c} \rangle_R - \langle \hat{c}^\dagger \rangle_R \langle \hat{d} \rangle_R) = 0 \] (137)

using Eqs. [131] and we see finally that the variances are

\[ \langle \Delta \hat{J}_x^2 \rangle_R = \frac{1}{4}(\langle \hat{d}^\dagger \rangle_R + \langle \hat{c}^\dagger \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d} \rangle_R) \]

\[ \langle \Delta \hat{J}_y^2 \rangle_R = \frac{1}{4}(\langle \hat{d}^\dagger \rangle_R + \langle \hat{c}^\dagger \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d} \rangle_R) \] (138)

and therefore from Eq. [134]

\[ \langle \Delta \hat{J}_z^2 \rangle \geq \sum_R P_R \left( \frac{1}{4}(\langle \hat{d}^\dagger \rangle_R + \langle \hat{c}^\dagger \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d} \rangle_R) \right) \]

\[ \langle \Delta \hat{J}_z^2 \rangle \geq \sum_R P_R \left( \frac{1}{4}(\langle \hat{d}^\dagger \rangle_R + \langle \hat{c}^\dagger \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d} \rangle_R) \right) \] (139)

Now

\[ \langle \hat{J}_z \rangle = \sum_R P_R \frac{1}{2}(\langle \hat{d}^\dagger \rangle_R - \langle \hat{c}^\dagger \rangle_R) \] (140)

so that

\[ \frac{1}{2} \left| \langle \hat{J}_z \rangle \right| \leq \sum_R P_R \frac{1}{4}(\langle \hat{d}^\dagger \rangle_R - \langle \hat{c}^\dagger \rangle_R) \leq \sum_R P_R \frac{1}{4}(\langle \hat{d}^\dagger \rangle_R + \langle \hat{c}^\dagger \rangle_R) \]

and thus for any non-entangled state of modes \( \hat{c} \) and \( \hat{d} \)

\[ \langle \Delta \hat{J}_z^2 \rangle - \frac{1}{2} \left| \langle \hat{J}_z \rangle \right| \geq \sum_R P_R \frac{1}{4}(\langle \hat{d}^\dagger \rangle_R + \langle \hat{c}^\dagger \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d} \rangle_R) - \sum_R P_R \frac{1}{4}(\langle \hat{d}^\dagger \rangle_R + \langle \hat{c}^\dagger \rangle_R) \]

\[ \geq \sum_R P_R \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d} \rangle_R) \]

\[ \geq 0 \] (141)

Similar final steps show that \( \langle \Delta \hat{J}_y^2 \rangle - \frac{1}{2} \left| \langle \hat{J}_z \rangle \right| \geq 0 \) for any non-entangled state of modes \( \hat{c} \) and \( \hat{d} \).

This shows that for the general non-entangled state with modes \( \hat{c} \) and \( \hat{d} \) as the sub-systems, the variances for two of the principal spin fluctuations \( \langle \Delta \hat{J}_x^2 \rangle \) and \( \langle \Delta \hat{J}_y^2 \rangle \) are both greater than \( \frac{1}{2} \left| \langle \hat{J}_z \rangle \right| \), and hence there is no spin squeezing for
\( \hat{J}_x \) or \( \hat{J}_y \). Note that as |\( \langle \hat{J}_y \rangle \)| = 0, the quantity \( \sqrt{(|\langle \hat{J}_{1.1} \rangle|^2 + |\langle \hat{J}_{1.2} \rangle|^2)} \) is the same as |\( \langle \hat{J}_z \rangle \)|, so the alternative criterion in Eq. (120) is the same as that in Eq. (116) which is used here.

We can extend the above to obtain further inequalities for the non-entangled state. Using Eq. (137)

\[
\langle \hat{J}_x \rangle = \sum_R P_R \langle \hat{J}_x \rangle_R = 0 \quad \langle \hat{J}_y \rangle = \sum_R P_R \langle \hat{J}_y \rangle_R = 0
\]  

it is easy to see that

\[
\langle \Delta \hat{J}_x^2 \rangle - \frac{1}{2} |\langle \hat{J}_y \rangle| \geq 0 \quad \langle \Delta \hat{J}_y^2 \rangle - \frac{1}{2} |\langle \hat{J}_x \rangle| \geq 0
\]

for any non-entangled state of modes \( \hat{c} \) and \( \hat{d} \). This completes the set of inequalities for the variances of \( \hat{J}_x \) and \( \hat{J}_y \).

### 4.1.2 Case of \( \hat{J}_z \)

For the other principal spin fluctuation we find that

\[
\langle \Delta \hat{J}_z^2 \rangle_R = \frac{1}{4} \left\langle \left( \hat{d} \hat{d} - \langle \hat{d} \hat{d} \rangle_R \right) \left( \hat{d} \hat{d} - \langle \hat{d} \hat{d} \rangle_R \right) \right\rangle_R + \langle \langle \hat{c}^\dagger \hat{c} - \langle \hat{c}^\dagger \hat{c} \rangle_R \rangle \rangle_R \]

so that using (137)

\[
\langle \Delta \hat{J}_z^2 \rangle \geq \sum_R P_R \frac{1}{4} \left\langle \left( \hat{d} \hat{d} - \langle \hat{d} \hat{d} \rangle_R \right)^2 \right\rangle_R + \langle \langle \hat{c}^\dagger \hat{c} - \langle \hat{c}^\dagger \hat{c} \rangle_R \rangle \rangle_R
\]

From Eq. (143) it follows that

\[
\langle \Delta \hat{J}_z^2 \rangle - \frac{1}{2} |\langle \hat{J}_x \rangle| \geq \sum_R P_R \frac{1}{4} \left\langle \left( \hat{d} \hat{d} - \langle \hat{d} \hat{d} \rangle_R \right)^2 \right\rangle_R + \langle \langle \hat{c}^\dagger \hat{c} - \langle \hat{c}^\dagger \hat{c} \rangle_R \rangle \rangle_R \geq 0
\]

Similarly \( \langle \Delta \hat{J}_y^2 \rangle - \frac{1}{2} |\langle \hat{J}_x \rangle| \geq 0 \).

### 4.1.3 No Spin Squeezing for Non-Entangled States

So overall, we have for the general non-entangled state of modes \( \hat{c} \) and \( \hat{d} \)

\[
\langle \Delta \hat{J}_x^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_x \rangle| \quad \langle \Delta \hat{J}_y^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_y \rangle| \quad \langle \Delta \hat{J}_z^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_z \rangle|
\]

\[
\langle \Delta \hat{J}_x^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_x \rangle| \quad \langle \Delta \hat{J}_y^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_y \rangle| \quad \langle \Delta \hat{J}_z^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_z \rangle|
\]
Note that the last two pairs of inequalities are trivially true for the general non-entangled state, since \( \langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0 \). This overall result tells us that for any non-entangled state of modes \( \hat{c} \) and \( \hat{d} \) we do not have \( \hat{J}_x \) being squeezed compared to \( \hat{J}_y \) (or vice-versa), \( \hat{J}_y \) being squeezed compared to \( \hat{J}_z \) (or vice-versa), \( \hat{J}_z \) being squeezed compared to \( \hat{J}_x \) (or vice-versa). That is, there is no spin squeezing for the non-entangled state!

4.1.4 Spin Squeezing Tests for Entanglement

The key value of these results is the spin squeezing test for entanglement - if for a given state we find that

\[
\text{If } \langle \Delta \hat{J}_x^2 \rangle < \frac{1}{2} |\langle \hat{J}_x \rangle| \quad \text{or} \quad \langle \Delta \hat{J}_y^2 \rangle < \frac{1}{2} |\langle \hat{J}_y \rangle| \tag{149}
\]

or

\[
\text{or } \langle \Delta \hat{J}_y^2 \rangle < \frac{1}{2} |\langle \hat{J}_y \rangle| \quad \text{or} \quad \langle \Delta \hat{J}_z^2 \rangle < \frac{1}{2} |\langle \hat{J}_z \rangle| \tag{150}
\]

or

\[
\text{or } \langle \Delta \hat{J}_z^2 \rangle < \frac{1}{2} |\langle \hat{J}_z \rangle| \quad \text{or} \quad \langle \Delta \hat{J}_x^2 \rangle < \frac{1}{2} |\langle \hat{J}_x \rangle| \tag{151}
\]

then the state must be entangled. Thus we only need to have spin squeezing in any of the \( \hat{J}_x, \hat{J}_y \) or \( \hat{J}_z \) to demonstrate entanglement. No particular component need be singled out. Note that one cannot have both \( \langle \Delta \hat{J}_x^2 \rangle < \frac{1}{2} |\langle \hat{J}_x \rangle| \) and \( \langle \Delta \hat{J}_y^2 \rangle < \frac{1}{2} |\langle \hat{J}_y \rangle| \) etc. due to the Heisenberg uncertainty principle.

It is then straightforward to show that

\[
\text{If } \langle \Delta \hat{J}_x^2 \rangle < \frac{1}{2} \sqrt{|\langle \hat{J}_{x,1} \rangle|^2 + |\langle \hat{J}_{x,2} \rangle|^2} \tag{152}
\]

or

\[
\text{or } \langle \Delta \hat{J}_y^2 \rangle < \frac{1}{2} \sqrt{|\langle \hat{J}_{y,1} \rangle|^2 + |\langle \hat{J}_{y,2} \rangle|^2} \tag{153}
\]

or

\[
\text{or } \langle \Delta \hat{J}_z^2 \rangle < \frac{1}{2} \sqrt{|\langle \hat{J}_{z,1} \rangle|^2 + |\langle \hat{J}_{z,2} \rangle|^2} \tag{154}
\]

that is, if \( \hat{J}_x, \hat{J}_y \) or \( \hat{J}_z \) are squeezed compared to any of their two orthogonal spin components - then the state must be entangled. Again we only need to have spin squeezing in any of the \( \hat{J}_x, \hat{J}_y \) or \( \hat{J}_z \) compared to any of their two orthogonal spin components to demonstrate entanglement.

4.1.5 Inequality for \( |\langle \hat{J}_z \rangle| \)

Of the results for a non-entangled physical state for modes \( \hat{c} \) and \( \hat{d} \) we will later find it particularly important to consider the first of (148)

\[
\langle \Delta \hat{J}_x^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_z \rangle| \quad \text{and} \quad \langle \Delta \hat{J}_y^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_z \rangle| \tag{155}
\]
This is because we can show that for any quantum state
\[
|\langle \hat{J}_z \rangle| = \left| \frac{1}{2} (\hat{n}_d - \hat{n}_c) \right| \leq \frac{1}{2} (|\langle \hat{n}_d \rangle| + |\langle \hat{n}_c \rangle|) = \frac{1}{2} \langle \hat{N} \rangle
\]  
(156)

there is an inequality involving \(|\langle \hat{J}_z \rangle|\) and the mean number of bosons \langle \hat{N} \rangle in the two mode system. Note that there may be entangled states for which \langle \Delta \hat{J}_x^2 \rangle and \langle \Delta \hat{J}_y^2 \rangle are both greater than \(\frac{1}{2}|\langle \hat{J}_z \rangle|\), since all that has been proven is that for non-entangled states we must have both \langle \Delta \hat{J}_x^2 \rangle \geq \frac{1}{2}|\langle \hat{J}_z \rangle|\) and \langle \Delta \hat{J}_y^2 \rangle \geq \frac{1}{2}|\langle \hat{J}_z \rangle|\).

Hence we may conclude that spin squeezing in either of the principal spin fluctuations \(\hat{J}_x\), \(\hat{J}_y\) or \(\hat{J}_z\) requires the quantum state to be entangled for the modes \(\hat{c}\) and \(\hat{d}\) as the sub-systems, these modes being associated with the principal spin fluctuations via Eq. (125). Although finding spin squeezing tells us that the state is entangled, there are however no simple relationships between the measures of entanglement and those of spin squeezing, so the linkage is essentially a qualitative one. For general quantum states, measures of entanglement for the specific situation of two sub-systems (bi-partite entanglement) are reviewed in [19].

4.2 Spin Squeezing requires Entanglement for Original Modes

It is also of some interest to consider spin squeezing for the original spin operators \(\hat{S}_x\), \(\hat{S}_y\), \(\hat{S}_z\) with the original modes \(\hat{a}\) and \(\hat{b}\) as the sub-systems, even though these spin operators are in general associated with a non-diagonal covariance matrix and the concept of spin squeezing is rather problematic in view of principal spin fluctuations not being involved. In this case the general non-entangled state for the original modes is given by
\[
\hat{\rho} = \sum_R P_R \hat{\rho}_R^A \otimes \hat{\rho}_R^B
\]  
(157)

with the \(\hat{\rho}_R^A\) and \(\hat{\rho}_R^B\) representing physical states for modes \(\hat{a}\) and \(\hat{b}\), and where results analogous to Eqs. (131) apply. The same treatment applies as for spin operators \(\hat{J}_x\), \(\hat{J}_y\), \(\hat{J}_z\) with the modes \(\hat{c}\) and \(\hat{d}\) as the sub-systems and leads to the result for a non-entangled state of modes \(\hat{a}\) and \(\hat{b}\)
\[
\langle \Delta \hat{S}_x^2 \rangle \geq \frac{1}{2} |\langle \hat{S}_z \rangle| \quad \text{and} \quad \langle \Delta \hat{S}_y^2 \rangle \geq \frac{1}{2} |\langle \hat{S}_z \rangle|
\]  
(158)

showing that neither \(\hat{S}_x\) or \(\hat{S}_y\) is spin squeezed for the general non-entangled state for modes \(\hat{a}\) and \(\hat{b}\) given in Eq. (157). We also have
\[
\langle \hat{S}_x \rangle = \sum_R P_R \langle \hat{S}_x \rangle_R = 0 \quad \langle \hat{S}_y \rangle = \sum_R P_R \langle \hat{S}_y \rangle_R = 0
\]  
(159)
so all the results analogous to Eqs. (148) also follow. Hence we may also conclude that spin squeezing in any of the original spin fluctuations requires the quantum state to be entangled when the original modes \( \hat{a} \) and \( \hat{b} \) are the sub-systems. Thus the entanglement test is

\[
\text{If } \langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_x \rangle| \quad \text{or} \quad \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} |\langle \hat{S}_y \rangle| \quad (160)
\]

or

\[
\text{If } \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} |\langle \hat{S}_x \rangle| \quad \text{or} \quad \langle \Delta \hat{S}_z^2 \rangle < \frac{1}{2} |\langle \hat{S}_y \rangle| \quad (161)
\]

or

\[
\text{If } \langle \Delta \hat{S}_z^2 \rangle < \frac{1}{2} |\langle \hat{S}_x \rangle| \quad \text{or} \quad \langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_y \rangle| \quad (162)
\]

then we have an entangled state for the original modes \( \hat{a} \) and \( \hat{b} \).

Hence we have seen that spin squeezing - either of the new or original spin operators requires entanglement of the new or original modes - the question then is: Does entanglement automatically lead to spin squeezing? The answer is no, since cases where the quantum state is entangled but not spin squeezed can be found. Thus in general, spin squeezing and entanglement are not equivalent - they do not occur together for all states. Spin squeezing is a sufficient condition for entanglement, it is not a necessary condition.

### 4.3 Entangled States that are Non Spin-Squeezed

One such example is the generalised \( N \) boson NOON state defined as

\[
\hat{\rho} = |\Phi\rangle \langle \Phi| = \cos \theta \frac{(\hat{c}^\dagger)^N}{\sqrt{N!}} |0\rangle + \sin \theta \frac{(\hat{d}^\dagger)^N}{\sqrt{N!}} |0\rangle = \cos \theta \left| \frac{N}{2}, -\frac{N}{2} \right\rangle + \sin \theta \left| \frac{N}{2}, \frac{N}{2} \right\rangle \quad (163)
\]

which is an entangled state for modes \( \hat{c} \) and \( \hat{d} \) in all cases except where \( \cos \theta \) or \( \sin \theta \) is zero. In the last form the state is expressed in terms of the eigenstates for \( (\hat{J}_x)^2 \) and \( \hat{J}_z \), as detailed in [65].

A straightforward calculation gives

\[
\begin{align*}
\langle \hat{J}_x \rangle &= 0 & \langle \hat{J}_y \rangle &= 0 & \langle \hat{J}_z \rangle &= -\frac{N}{2} \cos 2\theta \\
\langle \Delta \hat{J}_x^2 \rangle &= \frac{N}{4} & \langle \Delta \hat{J}_y^2 \rangle &= \frac{N}{4} & \langle \Delta \hat{J}_z^2 \rangle &= \frac{N^2}{4} (1 - \cos^2 2\theta) \quad (164)
\end{align*}
\]

for \( N > 1 \), so that using the criteria for spin squeezing given in Eq. (116) we see that as \( \langle \Delta \hat{J}_z^2 \rangle - \frac{1}{2} |\langle \hat{J}_z \rangle| \geq 0 \), etc, and hence spin squeezing does not occur for this entangled state.
4.4 Non-Entangled States that are Non Spin Squeezed

Of course from the previous section any non entangled state is definitely not spin squeezed. A specific example illustrating this is the $N$ boson binomial state given by

$$\hat{\rho} = |\Phi\rangle \langle\Phi|$$

$$|\Phi\rangle = \frac{(-\hat{c})^N}{\sqrt{N!}} |0\rangle$$

where $\hat{c}$ and $\hat{d}$ are given by Eqs. (127) with Euler angles $\alpha = -\pi + \chi, \beta = -2\theta$ and $\gamma = -\pi$, we find that

$$\hat{c} = -\cos \theta \exp\left(\frac{1}{2}i\chi\right) \hat{a} - \sin \theta \exp\left(-\frac{1}{2}i\chi\right) \hat{b} = -\hat{a}_1$$

$$\hat{d} = \sin \theta \exp\left(\frac{1}{2}i\chi\right) \hat{a} - \cos \theta \exp\left(-\frac{1}{2}i\chi\right) \hat{b} = -\hat{a}_2$$

where the mode operators $\hat{a}_1$ and $\hat{a}_2$ are as defined in [65] (see Eqs. (53) therein). The new spin angular momentum operators $\hat{J}_\xi (\xi = x, y, z)$ are the same as those defined in [65] (see Eqs. (64) therein) and in [65] it has been shown (see Eq. (60) therein) for the same binomial state as in (165) that

$$\langle \hat{J}_x \rangle = 0 \quad \langle \hat{J}_y \rangle = 0 \quad \langle \hat{J}_z \rangle = -\frac{N}{2}$$

$$\langle \Delta \hat{J}_x^2 \rangle = \frac{N}{4} \quad \langle \Delta \hat{J}_y^2 \rangle = \frac{N}{4} \quad \langle \Delta \hat{J}_z^2 \rangle = 0$$

(167)

(see Eqs. (162) and (176) therein). Hence the binomial state is not spin squeezed since $\langle \Delta \hat{J}_x^2 \rangle = \langle \Delta \hat{J}_y^2 \rangle = \frac{1}{4} \langle \hat{J}_z \rangle$. It is of course a minimum uncertainty state with spin fluctuations at the standard quantum limit. Clearly, it is a non-entangled state for modes $\hat{c}$ and $\hat{d}$, being the product of a number state for mode $\hat{c}$ with the vacuum state for mode $\hat{d}$.

Note that from the point of view of the original modes $\hat{a}$ and $\hat{b}$, this is an entangled state. So the question is: Is it a spin squeezed state with respect to the original spin operators $\hat{S}_\xi (\xi = x, y, z)$? The Bloch vector and variances for this binomial state are given in [65] (see Eq. (163) in the main paper and Eq. (410) in the Appendix). The results include:

$$\langle \hat{S}_z \rangle = -\frac{N}{2} \cos 2\theta$$

$$\langle \Delta \hat{S}_z^2 \rangle = \frac{N}{4} (\cos^2 2\theta \cos^2 \chi + \sin^2 \chi)$$

$$\langle \Delta \hat{S}_y^2 \rangle = \frac{N}{4} (\cos^2 2\theta \sin^2 \chi + \cos^2 \chi)$$

(168)

This gives $\langle \Delta \hat{S}_z^2 \rangle \langle \Delta \hat{S}_y^2 \rangle - \frac{1}{4} |\langle \hat{S}_z \rangle|^2 = \frac{1}{4} N^2 (\cos^2 2\theta - 1)^2 \cos^2 \chi \sin^2 \chi \geq 0$ as required for the Heisenberg uncertainty principle. With $\chi = 0$ we have
\[ \langle \Delta \hat{S}^2_x \rangle = \Delta \cos^2 \theta \quad \text{and} \quad \langle \Delta \hat{S}^2_y \rangle = \Delta \cos \theta, \quad \text{whilst} \quad \frac{1}{2} |\langle \hat{S}_z \rangle| = \Delta |\cos \theta|. \]

As \[ \langle \Delta \hat{S}^2_x \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle| \] there is spin squeezing in \( \hat{S}_x \) for this entangled state of modes \( \hat{a} \) and \( \hat{b} \), though not of course for the new spin operator \( \hat{J}_x \) since this state is non-entangled for modes \( \hat{c} \) and \( \hat{d} \). This example illustrates the need to carefully define spin squeezing and entanglement in terms of related sets of spin operators and modes. The same state is entangled with respect to one choice of modes - and spin squeezing occurs, whilst it is non-entangled with respect to another set of modes - and no spin squeezing occurs.

To summarise - with a physically based definition of non-entangled states for bosonic systems with two modes (related to the principal spin operators that have a diagonal covariance matrix) being the sub-systems and with a criterion for spin squeezing that focuses on these principal spin fluctuations, it seen that whilst non-entangled states are never spin squeezed and therefore although entanglement is a necessary condition for spin squeezing, it is not a sufficient one. There are entangled states that are not spin squeezed. Furthermore, as there is no simple quantitative links between measures of spin squeezing and those for entanglement, the mere presence of spin squeezing only demonstrates the qualitative result that the quantum state is entangled. Nevertheless, for high precision measurements based on spin operators where the primary emphasis is on how much spin squeezing can be achieved, knowing that entangled states are needed provides an impetus for studying such states and how they might be produced.

### 4.5 Entangled States that are Spin Squeezed

#### 4.5.1 Relative Phase Eigenstate

As an example of an entangled state that is spin squeezed we consider the relative phase eigenstate \( |N/2, \theta_p \rangle \) for a two mode system in which there are \( N \) bosons. For modes with annihilation operators \( \hat{a}, \hat{b} \) the relative phase eigenstate is defined as

\[
|N/2, \theta_p \rangle = \frac{1}{\sqrt{N+1}} \sum_{k=-N/2}^{N/2} \exp(i k \theta_p) \frac{\hat{a}^N \hat{b}^{N-k}}{\sqrt{(N/2-k)! (N/2+k)!}} |0\rangle
\]

where the relative phase \( \theta_p = p(2\pi/(N+1)) \) with \( p = -N/2, -N/2+1, ..., +N/2 \), is an eigenvalue of the relative phase Hermitian operator of the type introduced by Barnett and Pegg [79] (see [65] and references therein). Note that the eigenvalues form a quasi-continuum over the range \( -\pi \) to \( +\pi \), with a small separation between neighboring phases of \( O(1/N) \). The relative phase state is consistent with the super-selection rule and is an entangled state for modes \( \hat{a}, \hat{b} \). The Bloch vector for spin operators \( \hat{S}_x, \hat{S}_y, \hat{S}_z \) is given by (see [65])

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

but the covariance matrix (see Eq. (178) in [65]) is non-diagonal.
4.5.2 New Spin Operators

It is more instructive to consider spin squeezing in terms of new spin operators $\hat{J}_x, \hat{J}_y, \hat{J}_z$ for which the covariance matrix is diagonal. The new spin operators are related to the original spin operators via

$$
\hat{J}_x = \hat{S}_z, \quad \hat{J}_y = \sin \theta_p \hat{S}_x + \cos \theta_p \hat{S}_y, \quad \hat{J}_z = -\cos \theta_p \hat{S}_x + \sin \theta_p \hat{S}_y
$$

(171)
corresponding to the transformation in Eq. (113) with Euler angles $\alpha = -\pi + \theta_p$, $\beta = -\pi/2$ and $\gamma = -\pi$.

4.5.3 Bloch Vector and Covariance Matrix

The Bloch vector and covariance matrix for spin operators $\hat{J}_x, \hat{J}_y, \hat{J}_z$ are given by (see Eqs. (180), (181) in [65] - note that the $C(\hat{J}_y, \hat{J}_y)$ element is incorrect in Eq. (181))

$$
\langle \hat{J}_x \rangle = 0 \quad \langle \hat{J}_y \rangle = 0 \quad \langle \hat{J}_z \rangle = -N \frac{\pi}{8}
$$

(172)
and

$$
\begin{bmatrix}
C(\hat{J}_x, \hat{J}_x) & C(\hat{J}_x, \hat{J}_y) & C(\hat{J}_x, \hat{J}_z) \\
C(\hat{J}_y, \hat{J}_x) & C(\hat{J}_y, \hat{J}_y) & C(\hat{J}_y, \hat{J}_z) \\
C(\hat{J}_z, \hat{J}_x) & C(\hat{J}_z, \hat{J}_y) & C(\hat{J}_z, \hat{J}_z)
\end{bmatrix}
\begin{bmatrix}
\frac{1}{12} N^2 & 0 & 0 \\
0 & \frac{1}{4} + \frac{1}{8} \ln N & 0 \\
0 & 0 & \left(\frac{1}{6} - \frac{\pi^2}{64}\right) N^2
\end{bmatrix} N \gg 1
$$

(173)

With $\langle \Delta \hat{J}_x^2 \rangle = \frac{1}{12} N^2$, $\langle \Delta \hat{J}_y^2 \rangle = \frac{1}{4} + \frac{1}{8} \ln N$ and $\langle \Delta \hat{J}_z^2 \rangle = \left(\frac{1}{6} - \frac{\pi^2}{64}\right) N^2$ and the only non-zero Bloch vector component being $\langle \hat{J}_z \rangle = -N \frac{\pi}{8}$ it is easy to see that $\langle \Delta \hat{J}_x^2 \rangle \langle \Delta \hat{J}_y^2 \rangle \geq \frac{1}{4} \langle \hat{J}_z \rangle^2$ as required by the Heisenberg Uncertainty Principle. The principal spin fluctuations in both $\hat{J}_x$ and $\hat{J}_z$ are comparable to the length of the Bloch vector and no spin squeezing occurs in either of these components. However, spin squeezing occurs in that $\hat{J}_y$ is squeezed with respect to $\hat{J}_x$ - $\langle \Delta \hat{J}_y^2 \rangle$ only increases as $\frac{1}{8} \ln N$ whilst $\frac{1}{2} |\langle \hat{J}_z \rangle|$ increases as $\frac{\pi}{8} N$ for large $N$. Hence the relative phase state satisfies the test in Eq. (151) to demonstrate entanglement for modes $\hat{c}, \hat{d}$.

4.5.4 New Modes Operators

To confirm that the relative phase state is in fact an entangled state for modes $\hat{c}, \hat{d}$ as well as for the original modes $\hat{a}, \hat{b}$, we note that the new mode operators
\( \hat{c}, \hat{d} \) are given in in Eq. (127) with Euler angles \( \alpha = -\pi + \theta_p \), \( \beta = -\pi/2 \) and \( \gamma = -\pi \). The old mode operators are given in Eq. (129) and with these Euler angles we have

\[
\hat{a} = -\exp\left(\frac{1}{2}i\theta_p\right) \frac{1}{\sqrt{2}} (\hat{c} - \hat{d}) \\
\hat{b} = -\exp\left(-\frac{1}{2}i\theta_p\right) \frac{1}{\sqrt{2}} (\hat{c} + \hat{d})
\]

(174)

This enables us to write the phase state in terms of new mode operators \( \hat{c}, \hat{d} \) as

\[
\left| \frac{N}{2}, \theta_p \right> = \frac{1}{\sqrt{N + 1}} \left(\frac{-1}{\sqrt{2}}\right)^N \sum_{k = -N/2}^{N/2} \sum_{r = -N/4+k/2}^{N/4-k/2} \sum_{s = -N/4+k/2}^{N/4-k/2} \frac{1}{(N/2 - k)! (N/2 + k)! (-1)^{N/4-k/2+r}} \\
\times \frac{1}{(N/4-k/2-r)! (N/4-k/2+r)!} \frac{(N/2-k)!}{(N/2+k)!} \\
\times (\hat{c}^\dagger)^{N/2-(r+s)} (\hat{d}^\dagger)^{N/2+(r+s)} |0\rangle
\]

(175)

We see that the expression does not depend explicitly on the relative phase \( \theta_p \) when written in terms of the new mode unnormalised Fock states \( (\hat{c}^\dagger)^{N/2-(r+s)} (\hat{d}^\dagger)^{N/2+(r+s)} |0\rangle \). This pure state is a linear combination of product states of the form \( |N/2 - m\rangle_c \otimes |N/2 + m\rangle_d \) for various \( m \) - each of which is an \( N \) boson state and an eigenstate for \( \hat{J}_z \) with eigenvalue \( m \), and therefore is an entangled state for modes \( \hat{c}, \hat{d} \) which is compatible with the global super-selection rule. Note that there cannot just be a single term \( m \) involved, otherwise the variance for \( \hat{J}_z \) would be zero instead of \( 1/6 - \pi^2/64 \) \( N^2 \). We will return to the relative phase state again in SubSection 5.1.

### 4.6 Bloch Vector Entanglement Test

We have seen for the general non-entangled states of modes \( \hat{c} \) and \( \hat{d} \) or of modes \( \hat{a} \) and \( \hat{b} \) that

\[
\langle \hat{J}_x \rangle = 0 \quad \langle \hat{J}_y \rangle = 0 \quad (176) \\
\langle \hat{S}_x \rangle = 0 \quad \langle \hat{S}_y \rangle = 0 \quad (177)
\]

From Eqs. (126) and (111) these results are equivalent to

\[
\langle \hat{a} \hat{c}^\dagger \rangle = 0 \quad \langle \hat{c} \hat{d}^\dagger \rangle = 0 \quad (178) \\
\langle \hat{b} \hat{a}^\dagger \rangle = 0 \quad \langle \hat{a} \hat{b}^\dagger \rangle = 0 \quad (179)
\]

72
Hence we find further tests for entangled states of modes $\hat{c}$ and $\hat{d}$ or of modes $\hat{a}$ and $\hat{b}$

$$|\langle \hat{a} \hat{c} \rangle|^2 > 0 \quad |\langle \hat{c} \hat{d} \rangle|^2 > 0$$

$$|\langle \hat{b} \hat{a} \rangle|^2 > 0 \quad |\langle \hat{a} \hat{b} \rangle|^2 > 0$$

(180)  

(181)

As we will see in Section 5, these tests are particular cases with $m = n = 1$ of the simpler entanglement test in Eq. (205) that applies for the situation in the present paper where non-entangled states are required to satisfy the superselection rule.
5 Other Proposed Tests for Entanglement

There are a number of inequalities involving not only the variances of the spin operators but also other quantities, that have been derived for testing whether a state for a system of identical bosons is entangled. These are not always associated with criteria for spin squeezing. Some of these are based on the implicit assumption that the density operators $\hat{\rho}_A^R, \hat{\rho}_B^R$ in the expression for a non-entangled state are not required to conform to the super-selection rule that prohibits quantum superpositions of single mode states with differing numbers of bosons. These results are based in effect on a different criterion as to what constitutes an entangled state, so of course the resulting inequalities will differ from those that would apply if the definition of an entangled state is based on the considerations presented here in this paper - which emphasise the requirement that the density operators $\hat{\rho}_A^R, \hat{\rho}_B^R$ should represent physical states for the separate modes and hence satisfy the super-selection rule. Other results are based on forms of the density operator for non-entangled states that do not satisfy the symmetrisation principle. In this Section we examine a number of such entanglement tests and find that some are not valid, though some may be revised as tests for entangled states defined in accord with symmetrisation and super-selection rules.

5.1 Hillery et al 2006

5.1.1 Hillery Spin Variance Entanglement Test

One such entanglement test is presented in the paper by Hillery and Zubairy [32] entitled "Entanglement conditions for two-mode states". The paper actually dealt with EM field modes and the super-selection rule was not applied, so density operators $\hat{\rho}_A^R, \hat{\rho}_B^R$ for photon modes allowed for coherences between states with differing photon numbers, and hence the conditions in Eq. (131) did not apply. However, even for the situation of EM field modes where massless photons are involved, it is argued here that the super-selection rule also should be applied. Conditions involving the variances $\langle \Delta \hat{S}_x \rangle^2, \langle \Delta \hat{S}_y \rangle^2$ can be obtained by applying similar arguments to those in Section [5]. It is found that for the original spin operators $\hat{S}_x, \hat{S}_y, \hat{S}_z$ and modes $\hat{a}$ and $\hat{b}$

$$\langle \hat{S}_x^2 \rangle_R = \frac{1}{4} \langle \hat{b} \hat{b} \rangle_R^2 + \langle \hat{a} \hat{a} \rangle_R + \frac{1}{2} \langle \hat{b} \hat{a} \rangle \langle \hat{b} \hat{a} \rangle_R + \frac{1}{4} \langle \hat{b} \hat{b} \rangle_R^2 \langle \hat{a} \hat{a} \rangle_R + \langle \hat{b} \hat{b} \rangle_R^2 \langle \hat{a} \hat{a} \rangle_R$$

$$\langle \hat{S}_y^2 \rangle_R = \frac{1}{4} \langle \hat{b} \hat{b} \rangle_R^2 + \langle \hat{a} \hat{a} \rangle_R + \frac{1}{2} \langle \hat{b} \hat{a} \rangle \langle \hat{b} \hat{a} \rangle_R - \frac{1}{4} \langle \hat{b} \hat{b} \rangle_R^2 \langle \hat{a} \hat{a} \rangle_R + \langle \hat{b} \hat{b} \rangle_R^2 \langle \hat{a} \hat{a} \rangle_R$$

where terms such as $\langle \hat{b} \hat{b} \rangle_R^2$ and $\langle \hat{a} \hat{a} \rangle_R$ previously shown to be zero have been retained. Note that in [32] the operators $\hat{S}_x, \hat{S}_y, \hat{S}_z$, constructed from the EM field mode operators as in Eq. [111] would be related to Stokes parameters.
for any state

This inequality for non-entangled states is given in [32] (see Eq. (3)).

But from the Schwarz inequality - which is based on \( \langle \hat{a}^\dagger - \langle \hat{a} \rangle | \hat{a} - \langle \hat{a} \rangle \rangle \geq 0 \) for any state

so that that we now have

But from the Schwarz inequality - which is based on \( \langle \hat{a}^\dagger - \langle \hat{a} \rangle | \hat{a} - \langle \hat{a} \rangle \rangle \geq 0 \) for any state

so that

and thus from Eq. [134] it follows that for a general non entangled state

However, half the expectation value of the number operator is

so for a non-entangled state

This inequality for non-entangled states is given in [32] (see Eq. (3)). The above proof was based on a different definition of entangled states to that in this paper.
5.1.2 Validity of Hillery Test for Local SSR Compatible Non-Entangled States

However, it turns out that the same inequality is also valid when the definition of entangled states is the same as in the present paper. We would then find that
\[
\langle \hat{S}_x \rangle_R = \langle \hat{S}_y \rangle_R = 0
\]
and hence
\[
\langle \Delta \hat{S}_x^2 \rangle_R + \langle \Delta \hat{S}_y^2 \rangle_R = \frac{1}{2} \left( \langle \hat{b}^\dagger \hat{b} \rangle_R + \langle \hat{a}^\dagger \hat{a} \rangle_R \right) + \left( \langle \hat{b} \hat{b}^\dagger \rangle_R \right) (\langle \hat{a}^\dagger \hat{a} \rangle_R) \tag{192}
\]
instead of Eq. (186). Since the term \( \langle \hat{b}^\dagger \hat{b} \rangle_R \) \( (\langle \hat{a}^\dagger \hat{a} \rangle_R \) is always positive we find after applying Eq. (134) that
\[
\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq \frac{1}{2} \langle \hat{N} \rangle \tag{193}
\]
which is the same as in Eq. (191). Hence, finding that \( \langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} \langle \hat{N} \rangle \) would show that the state was entangled, irrespective of whether or not entanglement is defined in terms of non-physical unentangled states. The Hillery et al [32] entanglement test
\[
\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} \langle \hat{N} \rangle \tag{194}
\]
is still used in recent papers, for example [59], [80] which deal with the entanglement of sub-systems each consisting of single modes \( \hat{a}, \hat{b} \) for a double well situation (in these papers \( \hat{S}_x \rightarrow J_{AB}^X, \hat{S}_y \rightarrow -J_{AB}^Y, \hat{S}_z \rightarrow J_{AB}^Z \)).

5.1.3 Non-Applicable Entanglement Test Involving \( |\langle \hat{S}_z \rangle| \)

Previously we had found for a general non-entangled state that is based on physically valid density operators \( \hat{\rho}_R^A, \hat{\rho}_R^B \)
\[
\langle \Delta \hat{S}_x^2 \rangle - \frac{1}{2} |\langle \hat{S}_z \rangle| \geq 0
\]
\[
\langle \Delta \hat{S}_y^2 \rangle - \frac{1}{2} |\langle \hat{S}_z \rangle| \geq 0 \tag{195}
\]
so that the sum of the variances satisfies the inequality
\[
\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle| \tag{196}
\]
This is another correct inequality required for a non-entangled state as defined in the present paper. It follows that if only physical states \( \hat{\rho}_R^A, \hat{\rho}_R^B \) are allowed, the related entanglement test involving \( \langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \) would be
\[
\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < |\langle \hat{S}_z \rangle| \tag{197}
\]
For any quantum state we have

\[ |\langle \hat{S}_z \rangle | = \frac{1}{2} |\langle \hat{n}_b \rangle - \langle \hat{n}_a \rangle | \leq \frac{1}{2} |\langle \hat{n}_b \rangle + \langle \hat{n}_a \rangle | = \frac{1}{2} \langle \hat{N} \rangle \]  

(198)

which means that it is now required that \( \langle \Delta \hat{S}_z^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \) be less than a quantity that is smaller than in the criterion in (191).

However, it should be noted that all states, entangled or otherwise, satisfy the inequality \( \langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle | \) so the inequality in (196) - though true, is of no use in establishing whether a state is entangled in the terms of the meaning of entanglement in the present paper. There are no quantum states, entangled or otherwise that satisfy the proposed entanglement test given in Eq. (195). This general result was stated by Hillery et al. [32]. To show this we write the Heisenberg uncertainty principle for \( \langle \Delta \hat{S}_x^2 \rangle, \langle \Delta \hat{S}_y^2 \rangle \) as \( \langle \Delta \hat{S}_x^2 \rangle \langle \Delta \hat{S}_y^2 \rangle = \xi \frac{1}{2} |\langle \hat{S}_z \rangle |^2 \), where \( \xi \geq 1 \), then

\[
\frac{\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle}{|\langle \hat{S}_z \rangle |} = \frac{1}{2} \left( y + \frac{\xi}{y} \right) = F(y) \quad \text{where} \quad y = \frac{\langle \Delta \hat{S}_x^2 \rangle}{\frac{1}{2} |\langle \hat{S}_z \rangle |} \]  

(199)

It is straightforward to show that \( F(y) \geq 1 \) for all \( \xi, y \). The minimum value is 1, which occurs for \( \xi = 1 \) and \( y = 1 \). Even spin squeezed states with \( \langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle | \) still have \( \langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle | \), so it is never found that \( \langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < |\langle \hat{S}_z \rangle | \) and hence this latter inequality cannot be used as a test for entanglement.

Fortunately - as we have seen, showing that spin squeezing occurs via either \( \langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle | \) or \( \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle | \) is sufficient to establish that the state is an entangled state for modes \( \hat{a}, \hat{b} \), with analogous results if principle spin operators are considered. Applying the Hillery et al entanglement test in Eq. (194) involving \( \frac{1}{2} |\langle \hat{N} \rangle | \) is also a valid entanglement test, but is usually less stringent than the spin squeezing test involving either \( \langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle | \) or \( \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle | \). For the Hillery et al entanglement test to be satisfied at least one of \( \langle \Delta \hat{S}_x^2 \rangle \) or \( \langle \Delta \hat{S}_y^2 \rangle \) is required to be less than \( \frac{1}{2} |\langle \hat{N} \rangle | \), whereas for the spin squeezing test to apply at least one of \( \langle \Delta \hat{S}_x^2 \rangle \) or \( \langle \Delta \hat{S}_y^2 \rangle \) must be less than \( \frac{1}{4} |\langle \hat{S}_z \rangle | \). The quantity \( \frac{1}{2} |\langle \hat{S}_z \rangle | \) is likely to be smaller than \( \frac{1}{4} |\langle \hat{N} \rangle | \) - for example the Bloch vector may lie close to the \( xy \) plane, so a greater degree of reduction in spin fluctuation is needed to satisfy the spin squeezing test for entanglement.
However, this is not always the case as the example of the relative phase state discussed in SubSection 4.3 shows. The results in the current SubSection can easily be modified to apply to new spin operators $\hat{J}_x, \hat{J}_y, \hat{J}_z$, with entanglement being considered for new modes $\hat{c}$ and $\hat{d}$. The Hillery et al [32] entanglement test then becomes
\[
\left\langle \Delta \hat{J}_x^2 \right\rangle + \left\langle \Delta \hat{J}_y^2 \right\rangle < \frac{1}{2} \left\langle \hat{N} \right\rangle
\] (200)
In the case of the relative phase eigenstate we have from Eq. (173) that \( \left\langle \Delta \hat{J}_x^2 \right\rangle + \left\langle \Delta \hat{J}_y^2 \right\rangle = \frac{1}{12} N^2 + \frac{1}{4} + \frac{1}{2} \ln N \approx \frac{1}{12} N^2 \) for large N. This clearly exceeds \( \frac{1}{2} \left\langle \hat{N} \right\rangle = \frac{1}{2} N \), so the Hillery et al [32] test for entanglement fails. On the other hand, as we have seen in SubSection 4.3 \( \Delta \hat{J}_y^2 < \frac{1}{2} \left\langle \hat{J}_z \right\rangle \approx \frac{1}{16} N \), so the spin squeezing test is satisfied for this entangled state of modes $\hat{c}$ and $\hat{d}$.

5.2 Hillery et al 2009

5.2.1 Hillery Strong Correlation Entanglement Test

In a later paper entitled "Detecting entanglement with non-Hermitian operators" Hillery et al [33] apply other inequalities for determining entanglement derived in the earlier paper [32] but now also to systems of massive identical bosons, while still retaining density operators $\hat{\rho}_R$, $\hat{\rho}_R^\perp$ that contain coherences between states with differing boson numbers. In particular, for a non-entangled state the following family of inequalities - originally derived in [32], is invoked.
\[
|\left\langle \hat{a}^m (\hat{b})^n \right\rangle|^2 \leq \left\langle (\hat{\alpha}^\dagger)^m (\hat{\alpha})^m (\hat{\beta}^\dagger)^n (\hat{\beta})^n \right\rangle
\] (201)
Thus if \( |\left\langle \hat{a}^m (\hat{b})^n \right\rangle|^2 > \left\langle (\hat{\alpha}^\dagger)^m (\hat{\alpha})^m (\hat{\beta}^\dagger)^n (\hat{\beta})^n \right\rangle \) then the state is entangled.

A particular case for $n = m = 1$ is the test \( |\left\langle \hat{a} \hat{b}^\dagger \right\rangle|^2 > \left\langle \hat{n}_a \hat{n}_b \right\rangle \) for an entangled state. To put this result in context, for a general quantum state and any operator $\hat{\Omega}$ we have $\left\langle \hat{\Omega}^\dagger \right\rangle = \left\langle \hat{\Omega} \right\rangle^\dagger$ and $\left\langle \hat{\Omega}^\dagger - \left\langle \hat{\Omega} \right\rangle \right\rangle \left\langle \hat{\Omega} - \left\langle \hat{\Omega} \right\rangle \right\rangle \geq 0$, hence leading to the Schwarz inequality \( |\left\langle \hat{\Omega} \right\rangle|^2 = |\left\langle \hat{\Omega}^\dagger \right\rangle|^2 \leq \left\langle \hat{\Omega}^\dagger \hat{\Omega} \right\rangle \). Taking $\hat{\Omega} = \hat{a} \hat{b}^\dagger$ leads to the inequality \( |\left\langle \hat{a} \hat{b}^\dagger \right\rangle|^2 \leq \left\langle \hat{n}_a (\hat{n}_b + 1) \right\rangle \), whilst choosing $\hat{\Omega} = \hat{b} \hat{a}^\dagger$ leads to the inequality \( |\left\langle \hat{a} \hat{b}^\dagger \right\rangle|^2 \leq \left\langle (\hat{n}_a + 1) \hat{n}_b \right\rangle \) for all quantum states. In both cases the right side of the inequality is greater than $\left\langle \hat{n}_a \hat{n}_b \right\rangle$, so if it was found that \( |\left\langle \hat{a} \hat{b}^\dagger \right\rangle|^2 > \left\langle \hat{n}_a \hat{n}_b \right\rangle \) (though of course still $\leq \left\langle \hat{n}_a (\hat{n}_b + 1) \right\rangle$ and $\leq \left\langle (\hat{n}_a + 1) \hat{n}_b \right\rangle$) then it could be concluded that the state was entangled. However, as we will see the left side \( |\left\langle \hat{a} \hat{b}^\dagger \right\rangle|^2 \) actually works out to be zero if physical states for $\hat{\rho}_R$, $\hat{\rho}_R^\perp$ are involved in defining non-entangled states, so that for a non-entangled state defined as in the present paper the true inequality.
replacing \(|\langle \hat{a} \hat{b}^\dagger \rangle|^2 \leq (\hat{n}_a \hat{n}_b)\) is just 0 \(\leq (\hat{n}_a \hat{n}_b)\), which is trivially true for any quantum state. The test for entanglement requires modification.

The derivation of the general inequality in \[32\], as in Eq. \,(201) for a general non-entangled state of sub-systems \(A\) and \(B\). If we choose \(\hat{\Omega}_A = (\hat{a})^m\) and \(\tilde{\hat{\Omega}}_B = (\hat{\tilde{b}})^n\) then from \(|\langle \hat{\Omega}_A \otimes \tilde{\hat{\Omega}}_B \rangle|^2 \leq |\langle \hat{\Omega}_A \hat{\Omega}_A \otimes \tilde{\hat{\Omega}}_B \tilde{\hat{\Omega}}_B \rangle|\) the result of Hillery et al \[32\] stated in Eq. \,(201) immediately follows. The Hillery et al \[32\] entanglement test is that if

\[
|\langle (\hat{a})^m (\hat{b})^n \rangle|^2 > |\langle (\hat{a})^m (\hat{a})^m (\hat{b})^n (\hat{b})^n \rangle|
\]

then it may be concluded that the state is an entangled state for sub-systems \(A\) and \(B\). Note that the proof of this result did not depend on the sub-system density operators \(\hat{\rho}_A^R, \hat{\rho}_B^R\) being required to satisfy SSR.

5.2.2 Correlation Test for Entanglement for Local SSR Compatible Non-Entangled States

However, for a non-entangled state based on physical \(\hat{\rho}_A^R, \hat{\rho}_B^R\) for modes \(\hat{a}\) and \(\hat{\tilde{b}}\) where the SSR is satisfied we actually have

\[
|\langle (\hat{a})^m (\hat{b})^n \rangle|^2 = \sum_R P_R \langle (\hat{a})^m (\hat{b})^n \rangle_R = \sum_R P_R \langle (\hat{a})^m \rangle_R \langle (\hat{b})^n \rangle_R = 0
\]

since from Eqs. analogous to \[131\] \(|\langle (\hat{a})^m \rangle_R = \langle (\hat{b})^n \rangle_R = 0\). Hence for a physical non-entangled state as defined in the present paper the inequality becomes

\[
0 \leq |\langle (\hat{a})^m (\hat{\tilde{b}})^n (\hat{\tilde{b}})^n \rangle|
\]

which is trivially true and applies for any state, entangled or not.

Since \(|\langle (\hat{a})^m (\hat{\tilde{b}})^n \rangle|\) is zero for non-entangled states it follows that it is merely necessary to show that this quantity is non-zero to establish that the state is entangled. Hence an entanglement test in the case of sub-systems consisting of single modes \(\hat{a}\) and \(\hat{b}\) becomes

\[
|\langle (\hat{a})^m (\hat{b})^n \rangle|^2 > 0
\]

for a non-entangled state based on physical \(\hat{\rho}_A^R, \hat{\rho}_B^R\). This is a useful criterion for entanglement in terms the definition of entanglement in the present paper, and is different to that of Hillery et al \[32\]. The Hillery et al \[32\] entanglement test \(|\langle (\hat{a})^m (\hat{b})^n \rangle|^2 > |\langle (\hat{\tilde{a}})^m (\hat{\tilde{a}})^m (\hat{b})^n (\hat{b})^n \rangle|\) is also a valid test for entanglement and is actually a more stringent test than merely showing that \(|\langle (\hat{a})^m (\hat{b})^n \rangle|^2 > 0\), since the quantity \(|\langle (\hat{a})^m (\hat{b})^n \rangle|^2\) is now required to be larger. In a paper by He et al \[59\] (see Section IIIA) the Hillery et al \[32\] entanglement test \(|\langle (\hat{a})^m (\hat{b})^n \rangle|^2 > |\langle (\hat{\tilde{a}})^m (\hat{\tilde{a}})^m (\hat{b})^n (\hat{b})^n \rangle|\) is applied for the
case where \( A \) and \( B \) each consist of one mode localised in each well of a double well potential. This test whilst applicable could be replaced by the more easily satisfied test \( \left| \left\langle \hat{a}^m \hat{b}^n \right\rangle \right|^2 > 0 \). However, as will be seen below in SubSection 5.6 Hillery et al [32] entanglement criterion is needed if the sub-systems each consist of pairs of modes, as treated in [81], [59].

5.2.3 Examples Applying Correlation Tests for Entanglement

As an example of applying these tests consider the mixed two mode coherent states described in SubSection 2.13, whose density operator for the two mode \( \hat{a}, \hat{b} \) system is given in Eq. (104). We can now examine the Hillery et al [33] entanglement test in Eq.(202) and the entanglement test in Eq.(205) for the case where \( m = n = 1 \). It is straight-forward to show that

\[
\left| \left\langle \hat{a} \hat{b} \right\rangle \right|^2 = |\alpha|^4
\]

\[
\left\langle \hat{a}^\dagger \hat{a} \hat{b}^\dagger \hat{b} \right\rangle = |\alpha|^4
\]

so that \( \left| \left\langle \hat{a} \hat{b} \right\rangle \right|^2 = \left\langle \hat{a}^\dagger \hat{a} \hat{b}^\dagger \hat{b} \right\rangle \). A non-entangled state defined in terms of the SSR requirement for the separate modes satisfies \( \left| \left\langle \hat{a} \hat{b} \right\rangle \right|^2 = 0 \), whilst for a non-entangled state in which the SSR requirement for separate modes is not specifically required merely satisfies \( \left| \left\langle \hat{a} \hat{b} \right\rangle \right|^2 \leq \left\langle \hat{a}^\dagger \hat{a} \hat{b}^\dagger \hat{b} \right\rangle \). Hence the test for entanglement of modes \( A, B \) in the present paper \( \left| \left\langle \hat{a} \hat{b} \right\rangle \right|^2 > 0 \) is satisfied, whilst the Hillery et al [33] test \( \left| \left\langle \hat{a} \hat{b} \right\rangle \right|^2 \geq \left\langle \hat{a}^\dagger \hat{a} \hat{b}^\dagger \hat{b} \right\rangle \) is not.

In terms of the definition of non-entangled states in the present paper, the mixture of two mode coherent states given in Eq. (104) is an entangled state, not a separable state. However, in terms of the definition of non-entangled states in other papers such as those of Hillery et al [32], [33] the mixture of two mode coherent states would be a non-entangled state. It is thus a useful state for providing an example of the different outcomes of definitions where the local SSR is applied or not.

5.3 Sorensen et al 2001

5.3.1 Sorensen Spin Squeezing Entanglement Test

In a paper entitled "Many-particle entanglement with Bose-Einstein condensates" Sorensen et al [45] consider the implications for spin squeezing for non-entangled states of the form in Eq. (75). As discussed previously, a density operator of this general form is not consistent with the symmetrisation principle - having separate density operators \( \hat{\rho}_i \) for specific particles \( i \) in an identical particle system (such as for a BEC) is not compatible with the indistinguishability of such particles. It is modes that are distinguishable, not identical particles,
so the basis for applying their results to systems of identical bosons is flawed. However, they derive an inequality for the spin variance \( \langle \Delta \hat{S}_z^2 \rangle \)

\[
\langle \Delta \hat{S}_z^2 \rangle \geq \frac{1}{N} \left( \langle \hat{S}_x^2 \rangle + \langle \hat{S}_y^2 \rangle \right)
\]  

(207)

that applies in the case of non-entangled states. Key steps in their derivation are stated in the Appendix to [45], but as the justification of these steps is not obvious for completeness the full derivation is given in Appendix 15 of the present paper. This inequality (207) establishes that if

\[
\xi^2 = \frac{\langle \Delta \hat{S}_z^2 \rangle}{\left( \langle \hat{S}_x^2 \rangle + \langle \hat{S}_y^2 \rangle \right)} < \frac{1}{N}
\]  

(208)

then the state is entangled, so that if the condition for spin squeezing analogous to that in Eq. (120) is satisfied, then entanglement is required if spin squeezing for \( \hat{S}_z \) to occur. Spin squeezing is then a test for entanglement in terms of their definition of an entangled state. Note that the condition (120) requires the Bloch vector to be in the \( xy \) plane and close to the Bloch sphere of radius \( N/2 \).

5.3.2 Revising Sorensen Spin Squeezing Entanglement Test - Localised Modes

The work of Sorensen et al really applies only when the individual spins are distinguishable. It is possible however to modify the work of Sorensen et al [45] to apply to a system of identical bosons in accordance with the symmetrisation and super-selection rules if the index \( i \) is re-interpreted as specifying different modes, for example modes localised on optical lattice sites \( i = 1, 2, \ldots, N \). Details are given in Appendix 16. With two single particle states \( a, b \) available on each site (these could be two different internal atomic states or two distinct spatial modes localised on the site) the modes would then be labelled \( |\phi_{\alpha i}\rangle \) with \( \alpha = a, b \). The mode orthogonality and completeness relations would then be

\[
\sum_{\alpha i} |\phi_{\alpha i}\rangle \langle \phi_{\alpha i}| = \hat{1}
\]  

(209)

With the particles now labelled \( K = 1, 2, 3, \ldots \) one can define spin operators in first quantization via

\[
\hat{S}_x = \sum_K \sum_i (|\phi_{b i}(K)\rangle \langle \phi_{a i}(K)| + |\phi_{a i}(K)\rangle \langle \phi_{b i}(K)|)/2
\]

\[
\hat{S}_y = \sum_K \sum_i (|\phi_{b i}(K)\rangle \langle \phi_{a i}(K)| - |\phi_{a i}(K)\rangle \langle \phi_{b i}(K)|)/2i
\]

\[
\hat{S}_z = \sum_K \sum_i (|\phi_{b i}(K)\rangle \langle \phi_{b i}(K)| - |\phi_{a i}(K)\rangle \langle \phi_{a i}(K)|)/2
\]  

(210)
In second quantization if the annihilation, creation operators for the modes $|\phi_{ai}\rangle$, $|\phi_{bi}\rangle$ are $\hat{a}_i$, $\hat{b}_i$ and $\hat{a}_i^\dagger$, $\hat{b}_i^\dagger$ respectively, then the Schwinger spin operators are just

$$
\hat{S}_x = \sum_i (\hat{b}_i^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{b}_i)/2 = \sum_i \tilde{S}_x^i
$$

$$
\hat{S}_y = \sum_i (\hat{b}_i^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{b}_i)/2i = \sum_i \tilde{S}_y^i
$$

$$
\hat{S}_z = \sum_i (\hat{b}_i^\dagger \hat{b}_i - \hat{a}_i^\dagger \hat{a}_i)/2 = \sum_i \tilde{S}_z^i
$$

(211)

It is easy to confirm that the overall spin operators $\hat{S}_\alpha$ and the spin operators $\hat{S}_i^\alpha$ for the separate pairs of modes $|\phi_{ai}\rangle$, $|\phi_{bi}\rangle$ (or $\hat{a}_i$, $\hat{b}_i$ for short) satisfy the same commutation rules as Sorensen et al [45] have for the overall spin operators and those for the separate particles. With this modification the non-entangled state in Eq. (75) could be interpreted as being a non-entangled state where the subsystems are actually pairs of modes $|\phi_{ai}\rangle$, $|\phi_{bi}\rangle$. In terms of the present paper the density operators $\tilde{\rho}_R$ would be restricted by the super-selection rule to statistical mixtures of states with specific total numbers $N_i$ of bosons in the pair of modes $|\phi_{ai}\rangle$, $|\phi_{bi}\rangle$. In terms of Fock states $|n_{ai}\rangle$, $|n_{bi}\rangle$ for this pair of modes the allowed quantum states for the sub-system will be

$$
|\Phi_{N_i}\rangle = \sum_{k=0}^{N_i} A_{k}^{N_i} |k\rangle_{ai} |N_i - k\rangle_{bi}
$$

(212)

so at this stage the general mixed physical state for the two mode system could be

$$
\tilde{\rho}_R = \sum_{N_i=0}^{\infty} \sum_{\Phi} P_{\Phi N_i} \sum_{k=0}^{N_i} \sum_{l=0}^{N_i} A_k^{N_i} (A_l^{N_i})^* |k\rangle_{ai} \langle l|_{ai} \otimes |N_i - k\rangle_{bi} \langle N_i - l|_{bi}
$$

(213)

This state has no coherences between states of the two mode subsystem with differing total boson number $N_i$ for the pair of modes. However this is still an entangled states for the two modes $|\phi_{ai}\rangle$, $|\phi_{bi}\rangle$, so the overall state in Eq. (75) is not a non-entangled state if the subsystems were to consist of all the distinct modes.

5.3.3 Revising Sorensen Spin Squeezing Entanglement Test - Separable State of All Modes

It is possible however to link spin squeezing and entanglement in the case where the sub-systems consist of all the distinct modes. To obtain a fully non-entangled...
state of all the modes $|\phi_{ai}\rangle, |\phi_{bi}\rangle$ the density operator $\hat{\rho}_R^i$ must then be a product of density operators for modes $|\phi_{ai}\rangle$ and $|\phi_{bi}\rangle$

$$\hat{\rho}_R^i = \hat{\rho}_R^{a_i} \otimes \hat{\rho}_R^{b_i}$$

(214)

giving the full density operator as

$$\hat{\rho} = \sum_R P_R \left( \hat{\rho}_R^{a_1} \otimes \hat{\rho}_R^{b_1} \right) \otimes \left( \hat{\rho}_R^{a_2} \otimes \hat{\rho}_R^{b_2} \right) \otimes \left( \hat{\rho}_R^{a_3} \otimes \hat{\rho}_R^{b_3} \right) \otimes \ldots$$

(215)

as is required for a general non-entangled state all $2N$ modes. Furthermore, as previously the density operators for the individual modes must represent possible physical states for such modes, so the super-selection rule for atom number will apply and we have

$$\langle (\hat{a}_i)^n \rangle_{a_i} = Tr(\hat{\rho}_R^{a_i}(\hat{a}_i)^n) = 0 \quad \langle (\hat{a}_i)^n \rangle_{a_i} = Tr(\hat{\rho}_R^{a_i}(\hat{a}_i)^n) = 0$$

$$\langle (\hat{b}_i)^m \rangle_{b_i} = Tr(\hat{\rho}_R^{b_i}(\hat{b}_i)^m) = 0 \quad \langle (\hat{b}_i)^m \rangle_{b_i} = Tr(\hat{\rho}_R^{b_i}(\hat{b}_i)^m) = 0$$

(216)

The question is whether this reformulation will lead to a useful inequality for the spin variances such as $\langle \Delta \hat{S}_x^2 \rangle$. This issue is dealt with in Appendix 16 and it is found that we can indeed show for the general fully non-entangled state (215) that

$$\langle \Delta \hat{S}_x^2 \rangle \geq \frac{1}{2} |\langle \hat{S}_z \rangle| \quad \text{and} \quad \langle \Delta \hat{S}_y^2 \rangle \geq \frac{1}{2} |\langle \hat{S}_z \rangle|$$

(217)

This shows that if there is spin squeezing in either $\hat{S}_x$ or $\hat{S}_y$ then the state must be entangled. Note that this result depends on the general non-entangled state being non-entangled for all modes and that the density operator for each mode $\hat{a}_i$ or $\hat{b}_i$ being a physical state with no coherences between mode Fock states with differing atom numbers. In terms of the revised interpretation of the density operator to refer to a multi-mode system with modes $|\phi_{ai}\rangle, |\phi_{bi}\rangle$ the statement that spin squeezing for systems of identical massive bosons requires all the modes to be entangled is correct. However superposition states of the form (212) that are consistent with the super-selection rule applying to pure states of a two mode system are precluded, and such states ought to be allowed if entanglement of pairs of modes rather than of separate modes is to be considered.

5.3.4 Revising Sorensen Spin Squeezing Entanglement Test - Separable State of Pairs of Modes

It is also possible however to link spin squeezing and entanglement in the case where the subsystems consist of pairs of modes, but only if further restrictions are applied. The general non-entangled state of the pairs of modes would actually be of the form

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^{a_1} \otimes \hat{\rho}_R^{b_1} \otimes \hat{\rho}_R^{a_2} \otimes \hat{\rho}_R^{b_2} \otimes \ldots$$

(218)
where the $\hat{\rho}_R^i$ are now of the form given in Eq. (213) and no longer are density operators for the ith identical particle. Unlike in (210) we now have expectation values $(\langle \hat{a}_i \rangle^n)_i = Tr(\hat{\rho}_R^n(\hat{a}_i)^n)$ etc that are non-zero, so considerations of the link between spin squeezing and entanglement - now entanglement of pairs of modes, will be different.

If the density operators $\hat{\rho}_R^i$ associated with the pair of modes $\hat{a}_i, \hat{b}_i$ are all restricted to be associated with one boson states then this density operator is of the form

$$
\hat{\rho}_R^i = \rho_{aa}^i (|1\rangle_{ia} \langle 1|_{ia} \otimes |0\rangle_{ib} \langle 0|_{ib}) + \rho_{ab}^i (|1\rangle_{ia} \langle 0|_{ia} \otimes |0\rangle_{ib} \langle 1|_{ib}) + \rho_{ba}^i (|0\rangle_{ia} \langle 1|_{ia} \otimes |0\rangle_{ib} \langle 0|_{ib}) + \rho_{bb}^i (|0\rangle_{ia} \langle 0|_{ia} \otimes |1\rangle_{ib} \langle 1|_{ib})
$$

(219)

where the $\rho_{ef}^i$ are density matrix elements. With this restriction the pair of modes $\hat{a}_i, \hat{b}_i$ behave like distinguishable two state particles, essentially the case that Sorensen et al [45] implicitly considered. The expectation values $\langle \hat{S}_x^i \rangle_R, \langle \hat{S}_y^i \rangle_R, \langle \hat{S}_z^i \rangle_R$ for the restricted $n$-boson states willl be different.

If in addition Hermitiancy, positivity, unit trace $Tr(\hat{\rho}_R^i) = 1$ and $Tr(\hat{\rho}_R^i)^2 \leq 1$ are used (see Appendix 15) then we can show that $\rho_{ba}^i$ and $\rho_{aa}^i$ are real and positive, $\rho_{aa}^i = (\rho_{ba}^i)^*$ and $\rho_{aa}^i \rho_{bb}^i - |\rho_{ab}^i|^2 \geq 0$. The condition $Tr(\hat{\rho}_R^i) = 1$ leads to $\rho_{aa}^i + \rho_{bb}^i = 1$, from which $Tr(\hat{\rho}_R^i)^2 \leq 1$ follows using the previous positivity results. These results enable the matrix elements in (219) to be parameterised in the form

$$
\rho_{aa}^i = \sin^2 \alpha_i, \quad \rho_{bb}^i = \cos^2 \alpha_i,
$$

$$
\rho_{ab}^i = \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i \sin^2 \beta_i \exp(+i\phi_i)}, \quad \rho_{ba}^i = \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i \sin^2 \beta_i \exp(-i\phi_i)}
$$

(221)

where $\alpha_i, \beta_i, \phi_i$ are real. In terms of these quantities we then have

$$
\langle \hat{S}_x^i \rangle_R = \frac{1}{2} \sin 2\alpha_i \sin^2 \beta_i \cos \phi_i, \quad \langle \hat{S}_y^i \rangle_R = \frac{1}{2} \sin 2\alpha_i \sin^2 \beta_i \sin \phi_i, \quad \langle \hat{S}_z^i \rangle_R = \frac{1}{2} \cos 2\alpha_i
$$

(222)

and then a key inequality

$$
\langle \hat{S}_x^i \rangle_R^2 + \langle \hat{S}_y^i \rangle_R^2 + \langle \hat{S}_z^i \rangle_R^2 = \frac{1}{4} - \frac{1}{4} \sin^2 2\alpha_i (1 - \sin^4 \beta_i) \leq \frac{1}{4}
$$

(223)
follows. This result depends on the density operators $\hat{\rho}_R$ being for one boson states, as in (214). The same steps as in Sorensen et al [45] (see Appendix 15) leads to the result

$$\langle \Delta \hat{S}_z^2 \rangle \geq \frac{1}{N} \left( \langle \hat{S}_x \rangle^2 + \langle \hat{S}_y \rangle^2 \right)$$

(224)

for non-entangled pair of modes $\hat{a}_i, \hat{b}_i$. Thus when the interpretation is changed so that are the separate sub-systems are these pairs of modes and the sub-systems are in one boson states, it follows that spin squeezing requires entanglement of all the mode pairs.

A similar proof extending the test of Sorensen et al [45] to apply to systems of identical bosons is given by Hyllus et al [48] based on a particle entanglement approach. In their approach bosons in differing external modes (analogous to differing $i$ here) are treated as distinguishable, and the symmetrization principle is ignored for such bosons.

5.4 Sorensen and Molmer 2001

In a paper entitled "Entanglement and Extreme Spin Squeezing" Sorensen and Molmer [82] first consider the limits imposed by the Heisenberg uncertainty principle on the variance $\langle \Delta J_z^2 \rangle$ considered as a function of $|\langle \hat{J}_z \rangle|$ for states where the spin operators are chosen such that $\langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0$. Note that such spin operators can always be chosen so that the Bloch vector does lie along the $z$ axis, even if the spin operators are not principal spin operators. Their treatment is based on combining the result from the Schwarz inequality

$$\langle \hat{J}_x^2 \rangle + \langle \hat{J}_y^2 \rangle + \langle \hat{J}_z \rangle^2 \leq J(J+1)$$

(225)

where $J = N/2$, and the Heisenberg uncertainty principle

$$\langle \Delta \hat{J}_z^2 \rangle \langle \Delta \hat{J}_y^2 \rangle = \xi \frac{1}{4} |\langle \hat{J}_z \rangle|^2$$

(226)

where $\xi \geq 1$. In fact two inequalities can be obtained

$$\langle \Delta \hat{J}_x^2 \rangle \geq \frac{1}{2} \left\{ (J(J+1) - \langle \hat{J}_z \rangle^2) - \sqrt{(J(J+1) - \langle \hat{J}_z \rangle^2)^2 - \xi \langle \hat{J}_z \rangle^2} \right\}$$

(227)

$$\langle \Delta \hat{J}_x^2 \rangle \leq \frac{1}{2} \left\{ (J(J+1) - \langle \hat{J}_z \rangle^2) + \sqrt{(J(J+1) - \langle \hat{J}_z \rangle^2)^2 - \xi \langle \hat{J}_z \rangle^2} \right\}$$

(228)

which restricts the region in a $\langle \Delta \hat{J}_z^2 \rangle$ versus $|\langle \hat{J}_z \rangle|$ plane that applies for states that are consistent with the Heisenberg uncertainty principle. The first
of these two inequalities is given as Eq. (3) in [82]. For states in which $\hat{J}_x$ is squeezed relative to $\hat{J}_y$, the points in the $\langle \Delta \hat{J}_x^2 \rangle$ versus $\langle \hat{J}_z \rangle$ plane must also satisfy

$$\langle \Delta \hat{J}_x^2 \rangle \leq \frac{1}{2} |\langle \hat{J}_z \rangle|$$

(229)

Note that as $\hat{J}_z$ is a spin angular momentum component we always have $|\langle \hat{J}_z \rangle| \leq J$, which places an overall restriction on $|\langle \hat{J}_z \rangle|$. However, for $\xi > 1$ there are values of $|\langle \hat{J}_z \rangle|$ which are excluded via the Heisenberg uncertainty principle, since the quantity $\left( J(J+1) - \langle \hat{J}_z \rangle^2 \right)^2 - \xi \langle \hat{J}_z \rangle^2$ then becomes negative. This effect is seen in Figure 4.

The question is: Is it possible to find values for $\langle \Delta \hat{J}_x^2 \rangle$ and $|\langle \hat{J}_z \rangle|$ in which all three inequalities are satisfied? The answer is yes. Results showing the regions in the $\langle \Delta \hat{J}_x^2 \rangle$ versus $|\langle \hat{J}_z \rangle|$ plane corresponding to the three inequalities are shown in Figures 2 and 3 for the cases where $J = 1000$ and with $\xi = 1.0$ and $\xi = 10.0$ respectively. The quantities for which the regions are shown are the scaled variance and mean $\langle \Delta \hat{J}_x^2 \rangle/J$ and $|\langle \hat{J}_z \rangle|/J$, with $\langle \Delta \hat{J}_x^2 \rangle$ given as a function of $|\langle \hat{J}_z \rangle|$ via (227), (228) and (229). The spin squeezing region is always consistent with the second Heisenberg inequality (228) and for large $J = 1000$ there is a large region of overlap with the first inequality (227). For small $J$ and large $\xi$ the region of overlap becomes much smaller, as the result in Figure 4 for $J = 1$ and with $\xi = 10.0$ shows. As the derivation of the Heisenberg principle inequalities is not obvious, this is set out in Appendix 17.

Sorensen and Molmer [82] also determine the minimum for $\langle \Delta \hat{J}_x^2 \rangle = \langle \hat{J}_z^2 \rangle$ as a function of $|\langle \hat{J}_z \rangle|$ for various choices of $J$, subject to the constraints $\langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0$. The results show again that there is a region in the $\langle \Delta \hat{J}_x^2 \rangle$ versus $|\langle \hat{J}_z \rangle|$ plane which is compatible with spin squeezing.

So although these considerations show that the Heisenberg uncertainty principle does not rule out spin squeezing, nothing is determined about whether the spin squeezed states are entangled states for modes $\hat{c}$, $\hat{d}$, where the $\hat{J}_n$ are given as in Eq. (125). The discussion in [82] regarding entanglement is based on the physically incorrect density operator for non-entangled states of identical particles in Eq. (75), discussed in the previous section.

5.5 Duan et al 2000

A further inequality aimed at providing a signature for entanglement is set out in the papers by Duan et al [83], Toth et al [84]. For simplicity we only set out the case for which $a = 1$ in the former paper. This inequality involves position
and momentum like Hermitian operators defined by

\[ \hat{x}_A = \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger) \quad \hat{p}_A = \frac{1}{\sqrt{2}i}(\hat{a} - \hat{a}^\dagger) \]
\[ \hat{x}_B = \frac{1}{\sqrt{2}}(\hat{b} + \hat{b}^\dagger) \quad \hat{p}_B = \frac{1}{\sqrt{2}i}(\hat{b} - \hat{b}^\dagger) \]  

(230)

These are essentially quadrature operators and satisfy commutation rules \([\hat{x}_A, \hat{p}_A] = [\hat{x}_B, \hat{p}_B] = i\) similar to those for position and momentum. An inequality is obtained for a general two mode non-entangled state involving the variances for the commuting observables \(\hat{x}_A + \hat{x}_B\) and \(\hat{p}_A - \hat{p}_B\)

\[ \langle \Delta(\hat{x}_A + \hat{x}_B)^2 \rangle + \langle \Delta(\hat{p}_A - \hat{p}_B)^2 \rangle \geq 2 \]  

(231)

which could be used to establish a quadrature variance test for entangled states of the mode \(A\) and mode \(B\) sub-systems, so that if

\[ \langle \Delta(\hat{x}_A + \hat{x}_B)^2 \rangle + \langle \Delta(\hat{p}_A - \hat{p}_B)^2 \rangle < 2 \]  

(232)

then the modes are entangled. Such states are possible - consider for example any simultaneous eigenstate of the commuting observables \(\hat{x}_A + \hat{x}_B\) and \(\hat{p}_A - \hat{p}_B\). For such a state \(\langle \Delta(\hat{x}_A + \hat{x}_B)^2 \rangle\) and \(\langle \Delta(\hat{p}_A - \hat{p}_B)^2 \rangle\) are both zero, so the simultaneous eigenstates are entangled states of modes \(A, B\).

To confirm whether the inequality (231) applies for non-entangled states (231) in which the sub-system states \(\hat{\rho}^A_R, \hat{\rho}^B_R\) are physical, the general variance result in Eq. (134) plus the factorisations \(\langle \hat{x}_A\hat{x}_B \rangle_R = \langle \hat{x}_A \rangle_R \langle \hat{x}_B \rangle_R\) and \(\langle \hat{p}_A\hat{p}_B \rangle_R = \langle \hat{p}_A \rangle_R \langle \hat{p}_B \rangle_R\) are first used to show that

\[ \langle \Delta(\hat{x}_A + \hat{x}_B)^2 \rangle + \langle \Delta(\hat{p}_A - \hat{p}_B)^2 \rangle \geq \sum_R P_R \left( \langle \hat{x}_A^2 \rangle_R - \langle \hat{x}_A \rangle_R^2 + \langle \hat{x}_B^2 \rangle_R - \langle \hat{x}_B \rangle_R^2 + \langle \hat{p}_A^2 \rangle_R - \langle \hat{p}_A \rangle_R^2 + \langle \hat{p}_B^2 \rangle_R - \langle \hat{p}_B \rangle_R^2 \right) \]  

(233)

For sub-system states \(\hat{\rho}^A_R, \hat{\rho}^B_R\) that are physical we have in addition \(\langle \hat{x}_A \rangle_R = \langle \hat{x}_B \rangle_R = \langle \hat{p}_A \rangle_R = \langle \hat{p}_B \rangle_R = 0\). Also using \(\langle \hat{a}^2 \rangle_R = \langle (\hat{a}^\dagger)^2 \rangle_R = \langle \hat{b}^2 \rangle_R = \langle (\hat{b}^\dagger)^2 \rangle_R = 0\) for physical states we find for the remaining terms in Eq. (233) that

\[ \langle \hat{x}_A^2 \rangle_R = \frac{1}{2} \left( \langle \hat{a}^2 \rangle_R + \langle (\hat{a}^\dagger)^2 \rangle_R + 1 + 2 \langle \hat{a}^\dagger \hat{a} \rangle_R \right) \geq \frac{1}{2} \]
\[ \langle \hat{x}_B^2 \rangle_R = \frac{1}{2} \left( \langle \hat{b}^2 \rangle_R + \langle (\hat{b}^\dagger)^2 \rangle_R + 1 + 2 \langle \hat{b}^\dagger \hat{b} \rangle_R \right) \geq \frac{1}{2} \]
\[ \langle \hat{p}_A^2 \rangle_R = \frac{1}{2} \left( \langle \hat{a}^2 \rangle_R + \langle (\hat{a}^\dagger)^2 \rangle_R - 1 - 2 \langle \hat{a}^\dagger \hat{a} \rangle_R \right) \geq \frac{1}{2} \]
\[ \langle \hat{p}_B^2 \rangle_R = \frac{1}{2} \left( \langle \hat{b}^2 \rangle_R + \langle (\hat{b}^\dagger)^2 \rangle_R - 1 - 2 \langle \hat{b}^\dagger \hat{b} \rangle_R \right) \geq \frac{1}{2} \]  

(234)

87
Substituting these results into Eq. (233) establishes the validity of (231) for non-entangled states in which the \( \hat{\rho}_A \), \( \hat{\rho}_B \) are physical sub-system states. As there are entangled states that violate the inequality (231), this inequality is valid for determining whether a state is entangled.

### 5.6 He et al 2012

In two papers dealing with EPR entanglement He et al [81], [59] a four mode system associated with a double well potential is considered. In the left well \( A \) there are two localised modes with annihilation operators \( \hat{a}_1, \hat{a}_2 \) and in the right well \( B \) there are two localised modes with annihilation operators \( \hat{b}_1, \hat{b}_2 \). The modes in each well could be associated with different internal states or they could be associated with different spatial modes of the same internal state. This four mode system provides for the possibility of entanglement of two sub-systems each consisting of pairs of modes. With four modes there are three different choices of such sub-systems but perhaps the most interesting from the point of view of entanglement of spatially separated modes - and hence implications for EPR entanglement - would be to have the two left well modes \( \hat{a}_1, \hat{a}_2 \) as sub-system \( A \) and the two right well modes \( \hat{b}_1, \hat{b}_2 \) as sub-system \( B \). Consistent with the requirement that the sub-system density operators \( \hat{\rho}_A \), \( \hat{\rho}_B \) conform to the symmetrisation principle and the super-selection rule, these density operators may now be of the form given in Eq. (103). Hence as discussed in Sub-System 2.15 when considering non-entangled states for the sub-systems \( A \) and \( B \) we now have as in Eq. (110)

\[
\begin{align*}
\langle (\hat{a}_i)^n \rangle_A &= \text{Tr}(\hat{\rho}_R^A (\hat{a}_i)^n) \neq 0 \\
\langle (\hat{b}_j)^m \rangle_B &= \text{Tr}(\hat{\rho}_R^B (\hat{b}_j)^m) \neq 0
\end{align*}
\]

in general. Hence in this case where the sub-systems are pairs of modes the entanglement test in Eq. (205) for sub-systems consisting of single modes cannot be applied.

#### 5.6.1 Correlation Tests for Entanglement

However, the inequalities derived by Hillery et al [33] (see SubSection 5.2)

\[
| \langle (\hat{a}_i)^m (\hat{b}_j)^n \rangle |^2 \leq \langle (\hat{a}_i)^m (\hat{b}_j)^n \rangle \langle (\hat{b}_j)^n (\hat{b}_j)^n \rangle
\]

that apply for two non-entangled sub-systems \( A \) and \( B \) can now be usefully applied, since in this case the quantities \( \langle (\hat{a}_i)^m (\hat{b}_j)^n \rangle \) are in general no longer zero. Thus there is an entanglement test for two sub-systems consisting of pairs of modes. If

\[
| \langle (\hat{a}_i)^m (\hat{b}_j)^n \rangle |^2 > \langle (\hat{a}_i)^m (\hat{b}_j)^n \rangle \langle (\hat{b}_j)^n (\hat{b}_j)^n \rangle
\]

for any of \( i, j = 1, 2 \) (237)
then the quantum state for two sub-systems $A$ and $B$ - each consisting of two modes localised in each well - is entangled.

### 5.6.2 Spin Squeezing Tests for Entanglement

There are numerous choices for defining spin operators but the most useful would be the local spin operators for each well \[59\] defined by

$$
\hat{S}_x^A = (\hat{a}_1^2 + \hat{a}_2^2)/2 \quad \hat{S}_y^A = (\hat{a}_1^2 - \hat{a}_2^2)/2i \quad \hat{S}_z^A = (\hat{a}_2^1 - \hat{a}_1^1)/2
$$

$$
\hat{S}_x^B = (\hat{b}_1^2 + \hat{b}_2^2)/2 \quad \hat{S}_y^B = (\hat{b}_1^2 - \hat{b}_1^2)/2i \quad \hat{S}_z^B = (\hat{b}_2^1 - \hat{b}_1^1)/2
$$

(238)

These satisfy the usual angular momentum commutation rules and those or the different wells commute. The squares of the local vector spin operators are related to the total number operators $\hat{N}_A = \hat{a}_2^2 + \hat{a}_2^1$ and $\hat{N}_B = \hat{b}_2^2 + \hat{b}_1^2$ as $\sum(\hat{S}_A)^2 = (\hat{N}_A/2)(\hat{N}_A/2 + 1)$ and $\sum(\hat{S}_B)^2 = (\hat{N}_B/2)(\hat{N}_B/2 + 1)$.

For the local spin operators we have in general

$$
\langle \hat{S}_\alpha^A \rangle_A = Tr(\hat{\rho}_R^{\alpha} \hat{S}_\alpha^A) \neq 0 \quad \langle \hat{S}_\alpha^B \rangle_B = Tr(\hat{\rho}_R^{\alpha} \hat{S}_\alpha^B) \neq 0
$$

(239)

since the pair of modes $\hat{a}_1$, $\hat{a}_2$ and/or $\hat{b}_1$, $\hat{b}_2$ may now be of the form given in Eq. [103].

In SubSection 2.8 it was shown that $|\langle \hat{\Omega}_A^\dagger \hat{\Omega}_B \rangle|^2 \leq \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle$ for a non-entangled state, so with $\hat{\Omega}_A = \hat{S}_A^x - i\hat{S}_A^y$ and $\hat{\Omega}_B = \hat{S}_B^x - i\hat{S}_B^y = (\hat{S}_A^+)^\dagger$ to give

$$
|\langle \hat{S}_A^+ \hat{S}_B^- \rangle|^2 \leq |\langle \hat{S}_A^+ \hat{S}_-^A \hat{S}_+^B \hat{S}_-^B \rangle|
$$

(240)

for a non-entangled state of sub-systems $A$ and $B$. For the non-entangled state of these two sub-systems we have

$$
\langle \hat{S}_+^A \hat{S}_-^B \rangle = \sum_R P_R \langle \hat{S}_-^A \hat{S}_-^B \rangle = \sum_R P_R \langle \hat{S}_+^A \hat{S}_+^B \rangle
$$

(241)

which in general is non-zero from Eq. [239].

Hence a valid **entanglement test** involving spin operators for sub-systems $A$ and $B$ - each consisting of two modes localised in each well exists, and is if

$$
|\langle \hat{S}_+^A \hat{S}_-^B \rangle|^2 > |\langle \hat{S}_-^A \hat{S}_-^B \hat{S}_+^B \hat{S}_-^B \rangle|
$$

(242)

then the two sub-systems are entangled. A similar conclusion is stated in [59]. This test for entanglement involves the local spin operators, though it is not then the same as spin squeezing criteria. It is referred to as spin entanglement.
6 Experiments on Spin Squeezing

There are several papers [85], [86], [87] which contain the results of measuring the spin squeezing parameter analogous to the expression in Eq. (121) and showing that spin squeezing occurs. The presence of entanglement is then inferred by reference to theoretical papers such as [45] that show that spin squeezing only occurs for entangled states - it is an entanglement witness. As no independent measures of entanglement (however defined) are presented, nor are other independent tests for entanglement carried out, it cannot be said that these paper shows experimentally that spin squeezing requires entanglement. In [87] the emphasis is on showing how the spin squeezing can be generated via the non-linear terms in the Josephson Hamiltonian.
7 Discussion and Summary of Key Results

This paper is mainly concerned with two mode entanglement for systems of identical massive bosons and the relationship to spin squeezing. These bosons may be atoms or molecules as in cold quantum gases.

A careful analysis is first given regarding the proper definition of a non-entangled state for systems of identical particles, and hence by implication the proper definition of an entangled state. Noting that entanglement is meaningless until the subsystems being entangled are specified, it is pointed out that whereas it is not possible to distinguish identical particles and hence the individual particles are not legitimate sub-systems, the same is not the case for the single particle states or modes, so the modes are then the rightful sub-systems to be considered as being entangled or not. In this approach where the sub-systems are modes, situations where there are differing numbers of identical particles are treated as different physical states, not as differing physical systems, and the symmetrisation principle required of physical states for identical particle systems will be satisfied by using Fock states to describe the states.

Furthermore, it is argued that the overall physical states should conform to the superselection rule that excludes quantum superposition states of the form \( |\psi\rangle \) as physical states for systems of identical particles - massive or otherwise. Although the justification of the SSR in terms of observers and their reference frames formulated by other authors has also been presented for completeness, a number of fairly straightforward reasons were given for why it is appropriate to apply this superselection rule, which may be summarised as: 1. No way is known for creating such states. 2. No way is known for measuring all the properties of such states, even if they existed. 3. There is no need to invoke the existence of such states in order to understand coherence and interference effects. 4. The stability of such states against decoherence processes may not be great, so even if they could be created they could rapidly change to other states. The last reason is of lesser importance. Invoking the physical existence of states that as far as we know cannot be made or measured, and for which there are no known physical effects that require their presence seems a rather unnecessary feature to add to the non-relativistic quantum physics of many body systems, and considerations based on the general principle of simplicity (Occam’s razor) would suggest not doing this until a clear physical justification for including them is found. As two mode fermionic systems are restricted to states with at most two fermions, the focus of the paper is then on bosonic systems, where large numbers of bosons can occupy two mode systems.

However, although there is related work involving local particle number super-selection rules, this paper differs from a number of others by extending the super-selection rule to also apply to the density operators \( \hat{\rho}_A, \hat{\rho}_B, \ldots \) for the mode sub-systems \( A, B, \ldots \) that occur in the definition of a general non-entangled state for systems of identical particles. Hence it follows that the definition of entangled states will differ in this paper from that which would apply if density operators \( \hat{\rho}_A, \hat{\rho}_B, \ldots \) allowed for coherent superpositions of number states within each mode. In fact more states are regarded as entangled in
terms of the definition in the present paper. Indeed, if further restrictions are placed on the sub-system density operators - such as requiring them to specify a fixed number of bosons - the set of entangled states is further enlarged. The simple justification for our viewpoint on applying the local particle number super-selection rule has three aspects. Firstly, since experimental arrangements in which only one bosonic mode is involved can be created, the same reasons (see last paragraph) justify applying the super-selection rule to this mode system as applied for the system as a whole. Secondly, measurements can be carried out on the separate modes, and the joint probability for the outcomes of these measurements determined. For a non-entangled state the joint probability \( P_{AB..}(i,j,..) \) for measurements on all the sub-systems is given by the products of the individual sub-system probabilities \( P_A^{RI}(i) = Tr(\hat{\Pi}_A^i \hat{\rho}_A^R) \), etc that measurements on the sub-systems A, B,..yield the outcomes \( \lambda_i^A \) etc when the sub-systems are in states \( \hat{\rho}_A^R, \hat{\rho}_B^R, .. \), the overall products being weighted by the probability \( P_R \) that a particular product state is prepared. If \( \hat{\rho}_A^R, \hat{\rho}_B^R, \) did not represent physical states then the interpretation of the joint probability as this statistical average would be unphysical. Thirdly, attempts to allow the density operators \( \hat{\rho}_A^R, \hat{\rho}_B^R, .. \) for the mode sub-systems to violate the super-selection rule provided that the reduced density operators \( \hat{\rho}_A, \hat{\rho}_B \) for the separate modes are consistent with it are shown not to be possible in general.

As well as the above justifications for applying the super-selection rule to both the overall multi-mode state for systems of identical particles and the separate sub-system states in the definition of non-entangled states, a more sophisticated justification based on considering SSR to be the consequence of describing the quantum state by an observer (Charlie) whose phase reference is unknown has also been presented in detail in Appendix 12 for completeness. For the sub-systems local reference frames are involved. The SSR is seen as a special case of a general SSR which forbids quantum states from exhibiting coherences between states associated with irreducible representations of the transformation group that relates reference frames, and which may be the symmetry group for the system.

The present paper then defines spin squeezing for two mode systems and discusses the desirability of defining spin squeezing in terms of the principal spin operators \( \hat{J}_x, \hat{J}_y, \hat{J}_z \) for which the covariance matrix is diagonal, rather than via the original spin operators \( \hat{S}_x, \hat{S}_y, \hat{S}_z \) defined in terms of the original mode annihilation and creation operators \( \hat{a}, \hat{b} \) and \( \hat{a}^\dagger, \hat{b}^\dagger \) and for which the covariance matrix is non-diagonal in general. It is seen that the two sets of spin operators are related via a rotation operator and the principal spin operators are given in terms of new mode operators \( \hat{c}, \hat{d} \) and \( \hat{c}^\dagger, \hat{d}^\dagger \) with \( \hat{c}, \hat{d} \) obtained as linear combinations of the original mode operators \( \hat{a}, \hat{b} \) and hence defining two new
is not spin squeezed. Also, the binomial state NOON that though spin squeezing requires entanglement, the opposite is not the case such as the entanglement test ignores symmetrization or SSR. Hillery et al \cite{32} obtain criteria of this type, entangled from those involving spin squeezing that are obtained in this paper - hence entangled) states that is compatible with both these requirements.

On the other hand, the proof given here is based on a definition of non-entangled (and hence entangled) states that is entangled and spin squeezed for one choice of mode sub-systems may be non-entangled and not spin squeezed for another choice. The relative phase state provides an example that is entangled for new modes \( \hat{c}, \hat{d} \) and is highly spin squeezed in \( \hat{J}_y \) and very unsqueezed in \( \hat{J}_x \). The connection between spin squeezing and entanglement is regarded as well-known, but up to now only proofs based on non-entangled states that either disregard the symmetrization principle or the sub-system super-selection rules exist, placing the connection between spin squeezing and entanglement on a somewhat shaky basis. On the other hand, the proof given here is based on a definition of non-entangled (and hence entangled) states that is compatible with both these requirements.

There are several papers that obtain different tests for whether a state is entangled from those involving spin squeezing that are obtained in this paper, the proofs often being based on a definition of non-entangled states that ignores symmetrization or SSR. Hillery et al \cite{32} obtain criteria of this type, such as the entanglement test \( \langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} \langle \hat{N} \rangle \). This test is also valid if the non-entangled state definition is consistent with the SSR, but is different to the test \( \langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < |\langle \hat{S}_z \rangle| \) suggested by the requirement that \( \langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle| \) for non-entangled states - since both \( \langle \Delta \hat{S}_x^2 \rangle \geq |\langle \hat{S}_z \rangle|/2 \) and \( \langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle|/2 \). The latter inequality is of no use since \( \langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle| \) for all states. However as previously noted, showing that either \( \langle \Delta \hat{S}_x^2 \rangle < |\langle \hat{S}_z \rangle|/2 \) or \( \langle \Delta \hat{S}_y^2 \rangle < |\langle \hat{S}_z \rangle|/2 \) - or the analogous tests for other pairs of spin operators - already provides a test for the entanglement of the original modes \( \hat{a}, \hat{b} \). This test is a different test for entanglement than that of Hillery et al \cite{32}. The case of the relative phase eigenstate is an example of an entangled state in which the spin squeezing test for entanglement succeeds whereas that of Hillery et al \cite{32} fails.

Other inequalities found by Hillery et al \cite{33} for non-entangled states which also do not depend on whether non-entangled states satisfy the super-selection rule include \(| \langle \hat{a}^m (\hat{b}^l)^n \rangle |^2 \leq \langle \hat{a}^m (\hat{b}^l)^n \rangle \langle \hat{a}^m (\hat{b}^l)^n \rangle \), giving another valid test \(| \langle \hat{a}^m (\hat{b}^l)^n \rangle |^2 > \langle \hat{a}^m (\hat{b}^l)^n \rangle \langle \hat{a}^m (\hat{b}^l)^n \rangle \) for an entangled state. However, with
entanglement defined as in the present paper we have $|\langle \hat{a} \rangle^m (\hat{b}^\dagger)^n |^2 = 0$ for a non-entangled state, so an entanglement test in the form $|\langle \hat{a} \rangle^m (\hat{b}^\dagger)^n |^2 > 0$ immediately follows. This test is less stringent than that of Hillery et al [33], as $|\langle \hat{a} \rangle^m (\hat{b}^\dagger)^n |^2$ is then required to be larger. Sorensen et al [45] show that spin squeezing is a test for a state being entangled, but define non-entangled states for identical particle systems (such as BECs) in a form that is inconsistent with the symmetrisation principle - the sub-systems being regarded as individual identical particles. However, the treatment of Sorensen et al [45] can be modified to apply to a system of identical bosons if the particle index $i$ is re-interpreted as specifying different modes, for example modes localised on optical lattice sites $i = 1, 2, ..., N$. With two single particle states $|\phi_{ai}\rangle$, $|\phi_{bi}\rangle$ with annihilation operators $\hat{a}_i, \hat{b}_i$ available on each site, there would then be $2N$ modes involved, but spin operators can still be defined. If the definitions of non-entangled and entangled states in the present paper are applied, it can be shown that spin squeezing in either of the spin operators $\hat{S}_x$ or $\hat{S}_y$ requires entanglement of all the original modes $\hat{a}_i, \hat{b}_i$. Alternatively, if the sub-systems are pairs of modes $\hat{a}_i, \hat{b}_i$ and the sub-system density operators $\hat{\rho}_i$ were restricted to states with exactly one boson, then it can be shown that spin squeezing in $\hat{S}_z$ requires entanglement of all the pairs of modes. With this restriction the pair of modes $\hat{a}_i, \hat{b}_i$ behave like distinguishable two state particles, which was essentially the case that Sorensen et al [45] implicitly considered. This type of entanglement is a multi-mode entanglement of a special type - since the modes $\hat{a}_i, \hat{b}_i$ may themselves be entangled there is an "entanglement of entanglement". So with either of these key revisions, the work of Sorensen et al [45] could be said to show that spin squeezing requires entanglement. Sorensen and Mølmer [82] have deduced an inequality involving $\langle \Delta \hat{J}_z^2 \rangle$ and $|\langle \hat{J}_z \rangle|$ for states where $\langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0$ based on just the Heisenberg uncertainty principle. This is useful in terms of confirming that states do exist that are spin squeezed still conform to this principle. Duan et al [83], Toth et al [84] devise a test for entanglement based on the sum of the quadrature variances $\langle \Delta (\hat{x}_A + \hat{x}_B)^2 \rangle + \langle \Delta (\hat{p}_A - \hat{p}_B)^2 \rangle$, which involve quadrature components $\hat{x}_A, \hat{p}_A, \hat{x}_B, \hat{p}_B$ constructed from the original mode annihilation, creation operators for modes $A, B$. Their conclusion that if the sum is less than 2 then the state is entangled is valid both for the present definition of entanglement and for that in which the application of the super-selection rule is ignored. He et al [51], [59] consider a four mode system, with two modes localised in each well of a double well potential. If the two sub-systems $A$ and $B$ each consist of two modes - with $\hat{a}_1, \hat{a}_2$ as sub-system $A$ and $\hat{b}_1, \hat{b}_2$ as sub-system $B$, then tests of entanglement of the two sub-systems of the Hillery [33] type $|\langle \hat{a}_i \rangle^m (\hat{b}_j^\dagger)^n |^2 > |\langle \hat{a}_i \rangle^m (\hat{b}_i^\dagger)^n (\hat{b}_j^\dagger)^n |^2$ for any $i, j = 1, 2$ or involving local spin operators $|\langle \hat{S}_z^A \hat{S}_z^B \rangle |^2 > |\langle \hat{S}_z^A \hat{S}_z^B \rangle |^2$ apply.

Overall then, all of the entanglement tests (spin squeezing and other) in the other papers discussed here are still valid when reconsidered in accord with
the definition of entanglement based on the symmetrisation and super-selection rules, though in one case Sorensen et al. a re-definition of the sub-systems is required to satisfy the symmetrization principle. However, further tests for entanglement are obtained in the present paper based on non-entangled states that are consistent with the symmetrization and super-selection rules. In some cases they are less stringent - the correlation test in Eq.(210) being easier to satisfy than that of Hillery et al. in Eq. (202). They are certainly different to others previously discovered.

At present, experiments demonstrating spin squeezing do not show experimentally whether spin squeezing requires entanglement, however defined, since no results for entanglement measures are presented, nor are other independent tests for entanglement carried out.
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9 Appendix 1 - Projective Measurements and Conditional Probabilities

9.0.3 Projective Measurements

For simplicity, we will only consider projective (or von Neumann) measurements rather than more general measurements involving positive operator measurements (POM). If \( \hat{\Omega} \) is a physical quantity associated with the system, with eigenvalues \( \lambda_i \) and with \( \hat{\Pi}_i \) the projector onto the subspace with eigenvalue \( \lambda_i \), then the probability \( P(i) \) that measurement of \( \hat{\Omega} \) leads to the value \( \lambda_i \) is given by

\[
P(i) = Tr(\hat{\Pi}_i \hat{\rho})
\]  
(243)

For projective measurements \( \hat{\Pi}_i = \hat{\Pi}_i^2 = \hat{\Pi}_i^\dagger \) and \( \sum_i \hat{\Pi}_i = 1 \), together with \( \hat{\Omega} \hat{\Pi}_i = \hat{\Pi}_i \hat{\Omega} = \lambda_i \hat{\Pi}_i \).

Following the measurement which leads to the value \( \lambda_i \) the density operator is different and given by

\[
\hat{\rho}_{\text{cond}}(\hat{\Omega},i) = (\hat{\Pi}_i \hat{\rho} \hat{\Pi}_i)/P(i)
\]  
(244)

This is known as the reduction of the wave function, and can be viewed in two ways. From an ontological point of view a quantum projective measurement changes the quantum state significantly because the interaction with the measurement system is not just a small perturbation, as it can be in classical physics. From the epistomological point of view we know what value the physical quantity \( \hat{\Omega} \) now has, so if measurement of \( \hat{\Omega} \) were to be repeated immediately it would be expected - with a probability of unity - that the value would be \( \lambda_i \). The new density operator \( \hat{\rho}_{\text{cond}}(\hat{\Omega},i) \) satisfies this requirement. It also satisfies the standard requirements of Hermitiancy, unit trace, positivity - as is easily shown.

To show this formally we have for the mean value for \( \hat{\Omega} \) following the measurement

\[
\langle \hat{\Omega} \rangle_i = Tr(\hat{\Omega} \hat{\rho}_{\text{cond}}(\hat{\Omega},i))
\]  
(245)

\[
= Tr(\hat{\Omega} (\hat{\Pi}_i \hat{\rho} \hat{\Pi}_i))/P(i)
= \lambda_i Tr(\hat{\Pi}_i \hat{\rho} \hat{\Pi}_i)/P(i)
= \lambda_i
\]

whilst for the variance

\[
\langle \Delta \hat{\Omega}^2 \rangle_i = Tr((\hat{\Omega} - \langle \hat{\Omega} \rangle_i)^2 \hat{\rho}_{\text{cond}}(\hat{\Omega},i))
\]  
(246)

\[
= Tr(\hat{\Omega}^2 \hat{\rho}_{\text{red}}(i)) - \langle \hat{\Omega} \rangle_i^2
= \lambda_i^2 - \lambda_i^2
= 0
\]
which is zero as expected.

If following the measurement of $\hat{\Omega}$ the results of the measurement were discarded then the density operator after the measurement is

$$\hat{\rho}_{\text{cond}}(\hat{\Omega}) = \sum_i P(i) \hat{\rho}_{\text{cond}}(\hat{\Omega}, i) = \sum_i \hat{\Pi}_i \hat{\rho} \hat{\Pi}_i$$  \hspace{1cm} (247)

which is the sum of the $\hat{\rho}_{\text{cond}}(\hat{\Omega}, i)$ each weighted by the probability $P(i)$ of the result $\lambda_i$ occurring. Note that the expression for $\hat{\rho}_{\text{cond}}(\hat{\Omega})$ is not the same as the original density operator $\hat{\rho}$. This is to be expected from both the epistimological and ontological points of view, since although we do not know what value $\lambda_i$ has occurred, it is known that a definite value for $\hat{\Omega}$ has been found, or that measurement process has destroyed any coherences that previously existed between different eigenstates of $\hat{\Omega}$. We note that $\hat{\rho}_{\text{cond}}(\hat{\Omega})$ also satisfies the standard requirements of Hermitiancy, unit trace, positivity - as is easily shown.

### 9.0.4 Conditional Probabilities

Suppose we follow the measurement of $\hat{\Omega}$ resulting in eigenvalue $\lambda_i$ with a measurement of $\hat{\Lambda}$ resulting in eigenvalue $\mu_j$ where the projector associated with the latter measurement is $\hat{\Xi}_j$. Then the conditional probability of measuring $\hat{\Lambda}$ resulting in eigenvalue $\mu_j$ following the measurement of $\hat{\Omega}$ that resulted in eigenvalue $\lambda_i$ would be

$$P(j|i) = Tr(\hat{\Xi}_j \hat{\rho}_{\text{cond}}(\hat{\Omega}, i))$$

$$= Tr(\hat{\Xi}_j (\hat{\Pi}_i \hat{\rho} \hat{\Pi}_i))/P(i)$$

$$= Tr((\hat{\Xi}_j \hat{\Pi}_i) \hat{\rho} (\hat{\Pi}_i \hat{\Xi}_j))/P(i)$$  \hspace{1cm} (248)

where the cyclic properties of the trace and the idempotent property of the projector have been used. If the measurements had taken place in the reverse order the conditional probability of measuring $\hat{\Omega}$ resulting in eigenvalue $\lambda_i$ following the measurement of $\hat{\Lambda}$ that resulted in eigenvalue $\mu_j$ would be

$$P(i|j) = Tr((\hat{\Xi}_j \hat{\Pi}_i) \hat{\rho} (\hat{\Xi}_j \hat{\Pi}_i))/P(j)$$  \hspace{1cm} (249)

We note that the actual probability of measuring $\lambda_i$ then $\mu_j$ would be the joint probability

$$P(j \text{ after } i) = P(j|i) P(i) = Tr((\hat{\Xi}_j \hat{\Pi}_i) \hat{\rho} (\hat{\Pi}_i \hat{\Xi}_j))$$  \hspace{1cm} (250)

whilst the actual probability of measuring $\mu_j$ then $\lambda_i$ would be the joint probability

$$P(i \text{ after } j) = P(i|j) P(j) = Tr((\hat{\Xi}_j \hat{\Pi}_i) \hat{\rho} (\hat{\Xi}_j \hat{\Pi}_i))$$  \hspace{1cm} (251)

and we note that in general these two joint probabilities are different.

If however, the two physical quantities commute, then there are a complete set of simultaneous eigenvectors $\{|\lambda_i, \mu_j\rangle\}$ for $\hat{\Omega}$ and $\hat{\Lambda}$. It is then straightforward
to show that $\hat{\Pi}_i \hat{\Xi}_j = \hat{\Xi}_j \hat{\Pi}_i$, in which case $P(j \text{ after } i) = P(i \text{ after } j) = P(i,j)$, so it does not matter which order the measurements are carried out. The overall result

$$P(i,j) = P(j|i)P(i) = P(i|j)P(j)$$

$$= \text{Tr}(\hat{\Pi}_i \hat{\Xi}_j \hat{\rho} \hat{\Xi}_j \hat{\Pi}_i)$$

$$= \text{Tr}(\hat{\Pi}_i \hat{\Xi}_j \hat{\rho})$$

(252)

is an expression of Bayes theorem.

A case of particular importance where this occurs is in situations involving two or more distinct sub-systems, in which the operators $\hat{\Omega}$ and $\hat{\Lambda}$ are associated with different sub-systems. For two sub-systems $A$ and $B$ the operators $\hat{\Omega}$ and $\hat{\Lambda}$ are of the form $\hat{\Omega}_A \otimes \hat{1}_B$ and $\hat{1}_A \otimes \hat{\Omega}_B$. It is easy to see that $(\hat{\Omega}_A \otimes \hat{1}_B)(\hat{1}_A \otimes \hat{\Omega}_B) = \hat{\Omega}_A \otimes \hat{\Omega}_B = (\hat{1}_A \otimes \hat{\Omega}_B)(\hat{\Omega}_A \otimes \hat{1}_B)$, so the operators commute and results such as in Bayes theorem (252) apply.

9.0.5 Conditional Mean and Variance

To determine the conditioned mean value of $\hat{\Lambda}$ after measurement of $\hat{\Omega}$ has led to the eigenvalue $\lambda_i$ we use $\hat{\rho}_{\text{cond}}(\hat{\Omega},i)$ rather than $\hat{\rho}$ in the mean formula

$$\langle \hat{\Lambda} \rangle_i = \text{Tr}(\hat{\Lambda} \hat{\rho}_{\text{cond}}(\hat{\Omega},i))$$

Now

$$\hat{\Lambda} = \sum_j \mu_j \hat{\Xi}_j$$

(254)

so that

$$\langle \hat{\Lambda} \rangle_i = \sum_j \mu_j \text{Tr}(\hat{\Xi}_j \hat{\Pi}_i \hat{\rho} \hat{\Pi}_i) / P(i)$$

$$= \sum_j \mu_j \text{Tr}(\hat{\Xi}_j \hat{\Pi}_i \hat{\rho} \hat{\Pi}_i \hat{\Xi}_j) / P(i)$$

$$= \sum_j \mu_j P(j|i)$$

(255)

using $\hat{\Xi}_j = \hat{\Xi}_j^2$, the cyclic trace properties and Eq. (248). Hence the conditional mean value is as expected, with the conditional probability $P(j|i)$ replacing $P(j)$ in the averaging process.

For the conditioned variance of $\hat{\Lambda}$ after measurement of $\hat{\Omega}$ has led to the eigenvalue $\lambda_i$ we use $\hat{\rho}_{\text{cond}}(\hat{\Omega},i)$ rather than $\hat{\rho}$ and the conditioned mean $\langle \hat{\Lambda} \rangle_i$
rather than \( \langle \hat{\Lambda} \rangle \) in the variance formula \( \langle \Delta \hat{\Lambda}^2 \rangle = \text{Tr}((\hat{\Lambda} - \langle \hat{\Lambda} \rangle)^2 \tilde{\rho}) \). Hence

\[
\langle \Delta \hat{\Lambda}^2 \rangle_i = \text{Tr}((\hat{\Lambda} - \langle \hat{\Lambda} \rangle_i)^2 \tilde{\rho}_{\text{cond}}(\hat{\Omega}_i, i)) \\
= \text{Tr}((\hat{\Lambda} - \langle \hat{\Lambda} \rangle_i)^2 (\hat{\Pi}_i \hat{\rho} \hat{\Pi}_i))/P(i) \quad (256)
\]

Now

\[
(\hat{\Lambda} - \langle \hat{\Lambda} \rangle_i)^2 = \sum_j (\mu_j - \langle \hat{\Lambda} \rangle_{i,j})^2 \hat{\Xi}_j \quad (257)
\]

so that

\[
\langle \Delta \hat{\Lambda}^2 \rangle_i = \sum_j (\mu_j - \langle \hat{\Lambda} \rangle_{i,j})^2 \text{Tr}(\hat{\Xi}_j \hat{\Pi}_i \hat{\rho} \hat{\Pi}_i)/P(i) \\
= \sum_j (\mu_j - \langle \hat{\Lambda} \rangle_{i,j})^2 P(j|i) \quad (258)
\]

using the same steps as for the conditioned mean. Hence the conditional variance is as expected, with the conditional probability \( P(j|i) \) replacing \( P(j) \) in the averaging process.
10 Appendix 2 - Inequalities

These inequalities are examples of Schwarz inequalities.

10.1 Integral Inequality

If $C(\lambda), D(\lambda)$ are real, positive functions of $\lambda$ and $P(\lambda)$ is another real, positive function then we can show that

$$\int d\lambda P(\lambda)C(\lambda), \int d\lambda P(\lambda)D(\lambda) \geq \left(\int d\lambda P(\lambda)\sqrt{C(\lambda)D(\lambda)}\right)^2 \tag{259}$$

To show this write $x = \int d\lambda P(\lambda)C(\lambda)$ and $y = \int d\lambda P(\lambda)D(\lambda)$. Then

$$xy = \int d\lambda P(\lambda)C(\lambda) \int d\mu P(\mu)D(\mu) = \int \int d\lambda d\mu P(\lambda)P(\mu)C(\lambda)D(\mu)$$

$$= \int d\lambda P(\lambda)^2C(\lambda)D(\lambda) + \int d\lambda d\mu (1 - \delta(\lambda - \mu)) P(\lambda)P(\mu)\sqrt{C(\lambda)D(\lambda)\sqrt{C(\mu)D(\mu)}} \tag{260}$$

Also, write $z = \left(\int d\lambda P(\lambda)\sqrt{C(\lambda)D(\lambda)}\right)^2$. Then

$$z = \int d\lambda P(\lambda)\sqrt{C(\lambda)D(\lambda)} \int d\mu P(\mu)\sqrt{C(\mu)D(\mu)}$$

$$= \int \int d\lambda d\mu P(\lambda)P(\mu)\sqrt{C(\lambda)D(\lambda)}\sqrt{C(\mu)D(\mu)}$$

$$= \int d\lambda P(\lambda)^2C(\lambda)D(\lambda) + \int d\lambda d\mu (1 - \delta(\lambda - \mu)) P(\lambda)P(\mu)\sqrt{C(\lambda)D(\lambda)}\sqrt{C(\mu)D(\mu)}} \tag{261}$$

so that

$$xy - z = \int \int d\lambda d\mu (1 - \delta(\lambda - \mu)) P(\lambda)P(\mu) \left(C(\lambda)D(\mu) - \sqrt{C(\lambda)D(\lambda)\sqrt{C(\mu)D(\mu)}}\right)$$

$$= \frac{1}{2} \int \int d\lambda d\mu (1 - \delta(\lambda - \mu)) P(\lambda)P(\mu) \left(C(\lambda)D(\mu) + C(\mu)D(\lambda) - 2\sqrt{C(\lambda)D(\mu)\sqrt{C(\mu)D(\lambda)}}\right)$$

$$= \frac{1}{2} \int \int d\lambda d\mu (1 - \delta(\lambda - \mu)) P(\lambda)P(\mu) \left(\sqrt{C(\lambda)D(\mu)} - \sqrt{C(\mu)D(\lambda)}\right)^2 \geq 0 \tag{262}$$

which proves the result.

For the special case where $D(\lambda) = 1$ and where $\int d\lambda P(\lambda) = 1$ we get the simpler result

$$\int d\lambda P(\lambda)C(\lambda) \geq \left(\int d\lambda P(\lambda)\sqrt{C(\lambda)}\right)^2 \tag{263}$$

10.2 Sum Inequality

If $C_R$ and $D_R$ are real, positive quantities for various $R$ and $P_R$ is another real, positive quantity then we can show that

$$\sum_R P_R C_R \sum_R P_R D_R \geq \left(\sum_R P_R \sqrt{C_R D_R}\right)^2 \tag{264}$$
To prove this write \( x = \sum_{R} P_{R} C_{R} \) and \( y = \sum_{R} P_{R} D_{R} \).

Then

\[
xy = \sum_{R} P_{R} C_{R} \sum_{S} P_{S} D_{S} = \sum_{R} \sum_{S} P_{R} P_{S} C_{R} D_{S} = \sum_{R} P_{R}^{2} C_{R} D_{R} + \sum_{R} \sum_{S} (1 - \delta_{RS}) P_{R} P_{S} C_{R} D_{S} \tag{265}
\]

Also, write \( z = \left( \sum_{R} P_{R} \sqrt{C_{R} D_{R}} \right)^{2} \). Then

\[
z = \left( \sum_{R} P_{R} \sqrt{C_{R} D_{R}} \right) \left( \sum_{S} P_{S} \sqrt{C_{S} D_{S}} \right) = \sum_{R} \sum_{S} P_{R} P_{S} \sqrt{C_{R} D_{R} \sqrt{C_{S} D_{S}}} = \sum_{R} P_{R}^{2} C_{R} D_{R} + \sum_{R} \sum_{S} (1 - \delta_{RS}) P_{R} P_{S} \sqrt{C_{R} D_{R} \sqrt{C_{S} D_{S}}} \tag{266}
\]

so that

\[
xy - z = \sum_{R} \sum_{S} P_{R} P_{S} (1 - \delta_{RS}) \left( C_{R} D_{S} - \sqrt{C_{R} D_{R} \sqrt{C_{S} D_{S}}} \right) = \frac{1}{2} \sum_{R} \sum_{S} P_{R} P_{S} (1 - \delta_{RS}) \left( C_{R} D_{S} + C_{S} D_{R} - 2 \sqrt{C_{R} D_{S} \sqrt{C_{S} D_{R}}} \right) = \frac{1}{2} \sum_{R} \sum_{S} P_{S} P_{R} (1 - \delta_{RS}) \left( \sqrt{C_{R} D_{S}} - \sqrt{C_{S} D_{R}} \right)^{2} \geq 0 \tag{267}
\]

which proves the result.

For the special case where \( D_{R} = 1 \) and where \( \sum_{R} P_{R} = 1 \) we get the simpler result

\[
\sum_{R} P_{R} C_{R} \geq \left( \sum_{R} P_{R} \sqrt{C_{R}} \right)^{2} \tag{268}
\]

This inequality is used in [32].
11 Appendix 3 - Particle and Mode Entanglement

It is useful to contrast the two meanings of entanglement - mode and particle - in terms of three examples. The first is from the textbook by Peres [6], see pp126-128. A system with \( N = 2 \) identical particles has one particle in a single particle state (mode) \( |u\rangle \), the other in an orthogonal single particle state \( |v\rangle \). In first quantization the symmetrized quantum pure states for identical bosons or for identical fermions are (my notation) are

\[
|\Psi\rangle_{\text{boson}} = \frac{1}{\sqrt{2}}(|u(1)\rangle \otimes |v(2)\rangle + |u(2)\rangle \otimes |v(1)\rangle)
\]

\[
|\Psi\rangle_{\text{fermion}} = \frac{1}{\sqrt{2}}(|u(1)\rangle \otimes |v(2)\rangle - |u(2)\rangle \otimes |v(1)\rangle)
\]

which consequently means that "two particles of the same type are always entangled". Peres obviously considers such entanglement is a result of symmetrization. In second quantization the state in both the fermion and boson cases is \( |1\rangle_u \otimes |1\rangle_v \), which is a separable state for modes \( u, v \), and not a (mode) entangled state.

The second example is taken from the paper of Hyllus et al [48], specifically a case illustrated in Fig 1(b) which shows a state with \( N = 5 \) identical bosons. The bosons may occupy differing spatial states (eg harmonic oscillator states) - referred to by Hyllus et al as external degrees of freedom - and each bosonic particle has two distinct internal states (eg hyperfine states) - internal degrees of freedom. Fig 1(b) shows two spatial states and two internal states (\( u,d \) say), with only the lower spatial state (\( \phi_0 \) say) being occupied by \( N = 5 \) bosons. From the Hyllus et al viewpoint (see last para on p 012337-4) "For indistinguishable particles, only two possibilities are allowed in this case: either ALL the particles are in a separable state (that is, product \( |\phi\rangle^{\otimes N} \) state, or all particles are entangled due to the symmetrization." Hyllus et al describe the states in terms of first quantization but for purposes of comparison we will also describe them via second quantization. What they mean by the separable state is in full

\[
|\phi\rangle^{\otimes N} = |\phi_1\rangle |\phi_2\rangle |\phi_3\rangle |\phi_4\rangle |\phi_5\rangle
\]

where for the \( i \)th particle the single particle space-spin state would of the form

\[
|\phi_i\rangle = (\cos \theta |u_i\rangle + \sin \theta \exp i\chi |d_i\rangle) \otimes |\phi_{0i}\rangle
\]

in which a particular internal state is chosen. The separable state in Eq.(270) is just a tensor product of single particle states for the five bosons. It is symmetric, so the symmetrization principle is satisfied. There is of course one other orthogonal separable state \( |\xi\rangle^{\otimes N} = |\xi_1\rangle |\xi_2\rangle |\xi_3\rangle |\xi_4\rangle |\xi_5\rangle \) with an orthogonal single particle space-spin state \( |\xi_i\rangle = (-\sin \theta |u_i\rangle + \cos \theta \exp i\chi |d_i\rangle) \otimes |\phi_{0i}\rangle \) in which the internal state is orthogonal to the previous one. If one of the bosons is taken from a state \( |\phi\rangle \) and placed in the orthogonal state \( |\xi\rangle \), then representing it in
the form of a single tensor product such as \(|\phi_1\rangle |\phi_2\rangle |\phi_3\rangle |\phi_4\rangle |\xi_5\rangle\) would not satisfy the symmetrization principle. If one such product as \(|\phi_1\rangle |\phi_2\rangle |\phi_3\rangle |\phi_4\rangle |\xi_5\rangle\) is subjected to an operator which is the sum of all permutation operators \(\hat{P}\), then apart from normalising factor the result will represent the situation where one of the five bosons is in the state \(|\xi\rangle\) rather than \(|\phi\rangle\). Hence such a state is given by

\[
|\Psi_{4,1}\rangle = \mathcal{N} \sum_P \hat{P} (|\phi_1\rangle |\phi_2\rangle |\phi_3\rangle |\phi_4\rangle |\xi_5\rangle)
\]

which are where the sum is over the 5! permutation operators and the \(\mathcal{N}'s\) are normalising factors. However, Hyllus et al refer to this as entanglement by symmetrization and regard this state as being entangled. From this point of view it is symmetrization via \(\sum_P \hat{P}\) that is responsible for entanglement in that it creates contributions to the state vector which becomes no longer just a simple product. There is a term \(|\phi_1\rangle |\phi_2\rangle |\phi_3\rangle |\phi_4\rangle |\xi_5\rangle\) followed by \(|\phi_1\rangle |\phi_2\rangle |\phi_3\rangle |\xi_4\rangle |\phi_5\rangle\) in which particles 4 and 5 are in different single particle states.

However, from the opposing point of view in which it is modes, not particles that are entangled, and the state just described would not be regarded as being entangled. The Fig 1(b) case would be seen as a two mode situation in which the two modes are \(|U\rangle = |u\rangle \otimes |\phi_0\rangle\) and \(|D\rangle = |d\rangle \otimes |\phi_0\rangle\). In second quantization the Fock states are \(|n_U, n_D\rangle = |n_U\rangle \otimes |n_D\rangle\) with \(n_U, n_D\) being the mode occupancies. It is these two modes that may or may not be entangled, and there are six separable pure states (not two) with a total of \(N = 5\) bosons, namely \(|5, 0\rangle, |4, 1\rangle, |3, 2\rangle, |2, 3\rangle, |1, 4\rangle, \) and \(|0, 5\rangle\). The states \(|5, 0\rangle\) and \(|0, 5\rangle\) are of course equivalent in first quantization to \(|\phi_1\rangle |\phi_2\rangle |\phi_3\rangle |\phi_4\rangle |\phi_5\rangle\) and \(|\xi_1\rangle |\xi_2\rangle |\xi_3\rangle |\xi_4\rangle |\xi_5\rangle\), whilst the state in the last equation is just the separable state \(|4, 1\rangle\). The general mode entangled pure state with \(N = 5\) bosons is given by

\[
|\Psi\rangle = \mathcal{D}_{5,0} |5, 0\rangle + \mathcal{D}_{4,1} |4, 1\rangle + \mathcal{D}_{3,2} |3, 2\rangle + \mathcal{D}_{2,3} |2, 3\rangle + \mathcal{D}_{1,4} |1, 4\rangle + \mathcal{D}_{0,5} |0, 5\rangle
\]

where the \(\mathcal{D}\) are expansion coefficients, which is of course equivalent to various first quantization expressions. But now we would say it is the two modes \(|U\rangle\) and \(|D\rangle\) that are entangled, not the 5 bosons! Entanglement for \(N = 5\) boson pure states is associated with there being six distinct Fock states that occur for five bosons being split between two modes. If there were four modes then for \(N = 5\) boson pure states there would be many more distinct Fock states

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available depending on how the bosons are divided amongst the modes. It is more a question of *combinatorics* rather than *symmetrization* which is relevant in determining the *dimension* of the space of entangled states. A quite different picture of what is meant by an entangled state occurs when entanglement refers to modes rather than particles.
12 Appendix 4 - Reference Frames and Super-Selection Rules

Several papers such as [40], [42], [31], [34], [17], [35], [36] explain the link between reference frames and super-selection rules (SSR). In this Appendix we present the key ideas involved.

12.1 Two Observers and Reference Frames

The first point to appreciate is that there are two observers - Alice and Charlie - who are involved in describing the same state of a particular quantum system. Charlie is the external observer, Alice the internal observer - perhaps closely linked to the system. It is important to realise that it is Charlie’s description of the quantum state which is of most interest, in particular how this description may differ from what Alice may regard as the system state. The system could be a multi-mode system involving identical particles, it could just be a single mode system or it could even be a single particle with or without spin. Alice and Charlie each describe quantum states in terms of their own reference frames, which might be a set of coordinate axes for the case of the spin or position states for the single particle system, or it could be a large quantum system with a well-defined reference phase in the case of multi-mode or single mode systems involving identical particles. Alice and Charlie may each choose from a set of possible reference frames - for the single particle case there are an infinite number of difference choices of coordinate axes for example, related to each other via rotations and/or translations. In Situation A - which is not associated with SSR - Alice and Charlie do know the relationship between their two reference frames (and can communicate this relationship via classical communications) - such as in the case of the single particle system when the relative orientation of their two different coordinate axes are known. In Situation B - which is associated with SSR - Alice and Charlie do not know the relationship between their two reference frames - such as in the multi-mode or single mode system involving identical particles when the relative phase between their two large quantum phase reference systems is not known. Alice and Charlie describe the same state via density operators $\hat{\sigma}$ and $\hat{\rho}$, and the key question is the relationship between these two operators in situations A and B and for various types of reference frames. In terms of the notation in [31] $\rho \rightarrow \hat{\sigma}$ and $\tilde{\rho} \rightarrow \hat{\rho}$.

12.2 Symmetry Group

A particular relationship going from Alice’s to Charlie’s reference frame is specified by the parameter $g$, which in turn defines a unitary transformation operator $\hat{T}(g)$ that acts in the system space. Particular examples will be listed below. If there was a third observer - Donald - and the relationship going from Charlie’s to Donald’s reference frame is specified by the parameter $h$, which in turn defines a unitary operator $\hat{T}(h)$, then if we symbolise the relationship going from Alice’s to Donald’s reference frame by the parameter $hg$, it follows that...
$T(hg) = T(h)T(g)$. This shows that the unitary operators satisfy one of the requirements to constitute a group, referred to generally as the transformation group. The other requirements are easily confirmed. The unitary operator $T(0) = 1$ corresponding to the case where no change of reference frame occurs (specified by the parameter 0) exists, and satisfies the requirement that $T(0g) = T(0)T(g) = T(g0) = T(g)T(0)$. The unitary operator $T(g^{-1}) = T(g)^\dagger$ corresponding to the relationship specified as $g^{-1}$ that converts Charlie’s reference frame back to that of Alice exists, and satisfies the requirement that $T(0) = T(g^{-1})T(g) = T(g)T(g^{-1})$. Hence all the group properties are satisfied.

A few examples are as follows:

1. **Translation group** - single spinless particle system, with $\hat{p}$, $\hat{x}$ the momentum, position vector operators. Here $\vec{a}$ is a vector giving the translation of Charlie’s cartesian axes reference frame from that of Alice, thus $g \equiv \vec{a}$. The unitary translation operator is $\hat{T}(\vec{a}) = \exp(i\hat{p} \cdot \vec{a}/\hbar)$.

2. **Rotation group** - single particle system, with $\hat{J}$ the angular momentum vector operators. Here $\vec{u}$ is a unit vector giving the axis and rotation angle $\phi$ for rotating Alice’s cartesian axes reference frame into that of Charlie, thus $g \equiv \vec{u}, \phi$. The unitary rotation operator is $\hat{T}(\vec{u}, \phi) = \exp(i\phi \hat{J} \cdot \vec{u}/\hbar)$.

3. **Particle number U(1) group** - single mode bosonic system, with $\hat{a}$ the mode annihilation operator and $\hat{N}_a = \hat{a}^\dagger \hat{a}$ the mode number operator. Here $\theta_a$ is the phase change Alice’s to Charlie’s reference frame. The unitary operator is $\hat{T}(\theta_a) = \exp(i\hat{N_a} \theta_a)$.

4. **Particle number U(1) group** - multi-mode bosonic system, with $\hat{a}$ as a typical mode annihilation operator and $\hat{N} = \sum_a \hat{a}^\dagger \hat{a}$ the total number operator. Here $\theta$ is the phase change from Alice’s to Charlie’s reference frame. The unitary operator is $\hat{T}(\theta) = \exp(i\hat{N} \theta)$.

In these examples the system operators $\hat{p}$, $\hat{J}$, $\hat{N}_a$, $\hat{N}$ etc are the generators of the respective groups. In many situations the generators commute with the Hamiltonian for the system (or more generally with the evolution operator that describes time evolution of the quantum state), in which case the group of unitary operators $\hat{T}(g)$ is the symmetry group, and the generators are conserved physical quantities.

### 12.3 Relationships - Situation A

In *Situation A*, where the relationship between the reference frames for Alice and Charlie is known and specified by a single parameter $g$, Alice’s description of the state $\hat{\sigma}$ is related to Charlie’s description $\hat{\rho}$ for the same state via the unitary transformation

$$\hat{\rho} = \hat{T}(g) \hat{\sigma} \hat{T}(g)^{-1}$$  \hspace{1cm} (273)

Note that this is a passive transformation - no change of state is involved, just the same state being described by two different observers.
As an example, consider the spinless particle and the translation group. If $|\tilde{x}\rangle$ is a position eigenstate then $\tilde{T}(\tilde{a})|\tilde{x}\rangle = |\tilde{x} - \tilde{a}\rangle$. A pure quantum position eigenstate described by Alice as $\hat{\sigma} = |\Phi\rangle \langle \Phi|$ with state vector $|\Phi\rangle = |\tilde{x}\rangle$ would be described by Charlie as $\hat{\rho} = |\Psi\rangle \langle \Psi|$ but now with $|\Psi\rangle = |\tilde{x} - \tilde{a}\rangle$, which is also a pure quantum position eigenstate but with eigenvalue $\tilde{x} - \tilde{a}$. This is as expected since Alice’s cartesian axes have been translated by $\tilde{a}$ to the origin of Charlie’s axes without change of orientation. In the case of momentum eigenstates $|\tilde{p}\rangle$ we have $\tilde{T}(\tilde{a})|\tilde{p}\rangle = \exp(i \tilde{p} \cdot \tilde{a}/\hbar)|\tilde{p}\rangle$, so a pure momentum eigenstate described by Alice with $|\Phi\rangle = |\tilde{p}\rangle$ would be described by Charlie with $|\Psi\rangle = \exp(i \tilde{p} \cdot \tilde{a}/\hbar)|\tilde{p}\rangle$, which is also a pure momentum eigenstate with the same eigenvalue $\tilde{p}$. Alice and Charlie describe the pure momentum eigenstate with the same density operator $\hat{\rho} = \hat{\sigma}$, the phase factor cancels.

For more general pure states, consider a quantum state described by Alice as $\hat{\sigma} = |\Phi\rangle \langle \Phi|$ with state vector $|\Phi\rangle = \int \tilde{x} \phi(\tilde{x}) |\tilde{x}\rangle$. States of this form can represent localised states when $\phi(\tilde{x})$ is only significant in confined spatial regions, or they can represent delocalised states such as momentum eigenstates $|\tilde{p}\rangle$ when $\phi(\tilde{x}) = (2\pi\hbar)^{-3/2} \exp(i \tilde{p} \cdot \tilde{x}/\hbar)$. We see that Charlie also describes a pure quantum state $\hat{\rho} = |\Psi\rangle \langle \Psi|$ but now with $|\Psi\rangle = \tilde{T}(\tilde{a})|\Phi\rangle = \int \tilde{x} \phi(\tilde{x} + \tilde{a}) |\tilde{x}\rangle$, so the wavefunction is now $\psi(\tilde{x}) = \phi(\tilde{x} + \tilde{a})$.

Note that if Alice’s state vector was written in terms of momentum eigenstates $|\tilde{p}\rangle = \int \tilde{p} \phi(\tilde{p}) |\tilde{p}\rangle$, then Charlie’s state vector $|\Psi\rangle = \int \tilde{p} \psi(\tilde{p}) |\tilde{p}\rangle$ has a momentum wave function $\tilde{\psi}(\tilde{p}) = \exp(i \tilde{p} \cdot \tilde{a}/\hbar) \phi(\tilde{p})$ related to that of Alice by a phase factor. Note that a state which is a quantum superposition of momentum eigenstates as described by Alice is also described as a quantum superposition of momentum eigenstates by Charlie. A similar feature applies in all situation A cases, and is related to SSR not applying in situation A.

The case of the particle with spin and the rotation group is outlined in Ref. 12.

12.4 Relationships - Situation B

In Situation B, where on the other hand the relationship between frames is completely unknown, all possible transformations $g$ must be given equal weight, and hence the relationship between Alice’s and Charlie’s description of the same
state becomes
\[ \hat{\rho} = \int w(g) dg \hat{T}(g) \hat{\sigma} \hat{T}(g)^{-1} = \mathcal{G}[\hat{\sigma}] \]

(274)

where \( \int w(g) dg \) is a symbolic integral over the parameter \( g \), which includes a weight factor \( w(g) \) so that \( \int w(g) dg = 1 \). This linear process connecting \( \hat{\sigma} \) to \( \hat{\rho} \) is the "\( \mathcal{G} \)-twirling" operation. Again, this is a passive transformation.

It is straightforward to show that for any fixed parameter \( h \) that
\[ \hat{T}(h) \hat{\rho} \hat{T}(h)^{-1} = \hat{\rho} \]

(275)

showing that Charlie’s density operator is \( \mathcal{G} \) invariant under the transformation group - unlike the case for Situation A.

As an example, consider the single mode bosonic system and the \( U(1) \) group. If \( |n_a\rangle \) is a Fock state then \( \hat{T}(\theta_a) |n_a\rangle = \exp(i n_a \theta_a) |n_a\rangle \). Consider a pure quantum state described by Alice as the Glauber coherent state \( \hat{\sigma} = |\Phi\rangle \langle \Phi| \) with state vector \( |\Phi(\beta)\rangle = \sum_n C(n_a, \beta) |n_a\rangle \), where \( C(n_a, \beta) = \exp(-|\beta|^2/2) \beta^{n_a}/\sqrt{(n_a)!} \).

It is straightforward to show that
\[ \hat{T}(\theta_a) |\Phi(\beta)\rangle = |\Phi(\beta \exp(i \theta_a))\rangle \]

(276)

so that the Glauber coherent state is transformed into another Glauber coherent state, but with \( \beta \) changed via a phase factor to \( \beta \exp(i \theta_a) \). The quantum state described by Charlie is given by
\[ \hat{\rho} = \int \frac{d\theta_a}{2\pi} |\Phi(\beta \exp(i \theta_a))\rangle \langle \Phi(\beta \exp(i \theta_a))| \]

(277)

\[ = \int \frac{d\theta_a}{2\pi} \sum_{n_a} \sum_{m_a} C(n_a, \beta) C(m_a, \beta)^* \hat{T}(\theta_a) |m_a\rangle \langle n_a| \]

\[ = \sum_{n_a} \sum_{m_a} C(n_a, \beta) C(m_a, \beta)^* |n_a\rangle \langle m_a| \int \frac{d\theta_a}{2\pi} \exp(i |n_a - m_a| \theta_a) \]

\[ = \sum_{n_a} \exp(-|\beta|^2) \frac{(|\beta|^2)^{n_a}}{(n_a)!} |n_a\rangle \langle n_a| \]

(278)

which is a mixed state consisting of a Poisson distribution of Fock states with mean occupation number \( \bar{n}_a = |\beta|^2 \). In view of the first expression for \( \hat{\rho} \) it can also be thought of as a mixed state consisting of Glauber coherent states each with the same amplitude \( |\beta| = \sqrt{\bar{n}_a} \), but with all phases \( \arg(\beta + \theta_a) \) equally probable. Thus, whereas Alice describes the state as a pure state that
is a quantum superposition of Fock states with differing occupancy numbers, Charlie describes the same state as a mixed state involving a statistical mixture of number states. The former violates the SSR whereas the latter does not. A similar feature applies in all situation B cases, and is related to SSR applying in Situation B. Whether Alice could ever prepare such a state in the first place is controversial - see the discussion presented above in SubSections 2.10 and 2.12. However, assuming she could, the quantum state as described by Charlie is a mixed state.

The situation just studied relates of course to the debate [68] regarding whether the quantum state for a single mode laser operating well above threshold should be described by a Glauber coherent state or as a Poisson statistical mixture of photon number states. The first viewpoint (Alice) describes the state from the point of view of an internal observer with a reference frame, the second (Charlie) describes the same state from the point of view of an external observer for whose reference frame relationship to that of the internal observer is unknown. The debate is regarded by [42] as settled on the basis that both viewpoints are valid, they are just at cross purposes because they refer to descriptions of the same quantum state by two different observers.

It should not be thought however that the quantum state would always be described in such a fundamentally different manner for all Situation B cases. As an example, consider the multi-mode bosonic system and the $U(1)$ group. Consider the pure quantum state described by Alice as the multi-mode $N$ boson Fock state $\hat{\sigma} = |\Phi\rangle \langle \Phi|$, with state vector $|\Phi(N)\rangle = \prod_a |n_1\rangle |n_2\rangle \cdots |n_a\rangle \cdots$, where $N = \sum_a n_a$. We have $\hat{T}(\theta) |\Phi^\pm\rangle = \exp(i N \theta) |\Phi^\pm\rangle$, so that the same state would be described by Charlie as $\hat{\rho} = |\Psi\rangle \langle \Psi|$ and with $|\Psi\rangle = |n_1n_2\cdots n_a\cdots; N\rangle$. This is also a multi-mode $N$ boson Fock state with exactly the same occupancies. The product $\exp(i N \theta) \exp(-i N \theta)$ of phase factors averages out to unity and here $\hat{\rho} = \hat{\sigma}$, so Alice and Charlie both describe the multi-mode Fock states in the same way. Another example for two mode bosonic systems and the $U(1)$ group is provided by the one boson Bell states (the BS notation used here is non-conventional). These are entangled two mode states that Alice would describe via the state vectors $|\Phi^\pm\rangle = (|10\rangle \pm |01\rangle)/\sqrt{2}$. We have $\hat{T}(\theta) |\Phi^\pm\rangle = \exp(i \theta) |\Phi^\pm\rangle$, so that the same state would be described by Charlie with $|\Psi^\pm\rangle = (|10\rangle \pm |01\rangle)/\sqrt{2}$. Again the product of phase factors averages to unity and $\hat{\rho} = \hat{\sigma}$, so Alice and Charlie both describe the quantum states as Bell states, and in the same form.

12.5 Dynamical and Measurement Considerations

Discussions of the relationship between equations governing the dynamical behaviour of Alice’s and Charlie’s density operators depend on whether the evolution is just governed by a Hamiltonian or whether master equations describing evolution affected by interactions with an external environment are involved. Such matters will not be treated in detail here, nor will the issue of relating
Alice’s and Charlie’s measurements. The latter issue is dealt with in [31].

However, in the case where Alice describes the Hamiltonian evolution of her density operator via the Liouville-von-Neumann equation

\[
\frac{i\hbar}{\partial t} \sigma = [\hat{H}, \sigma]
\]

(279)

where in Alice’s frame the Hamiltonian is \( \hat{H} \), and where in addition the transformation group is also the symmetry group so that \( \hat{T}(g)\hat{H}\hat{T}(g)^{-1} = \hat{H} \) for all \( g \), it is easy to see that for both Situations A and B, Charlie’s density operator will evolve via the same LVN equation

\[
\frac{i\hbar}{\partial t} \rho = [\hat{H}, \rho]
\]

(280)

Thus both Alice and Charlie will describe the same dynamical evolution, though of course the initial (and hence evolved) states may differ in the two cases.

### 12.6 Nature of Reference Frames

Reference frames of differing types are involved for the various transformation groups. The common feature is that they are thought of as actual physical systems themselves which are either macroscopic classical systems or macroscopic quantum systems in states associated with the classical limit. They are intended to be essentially unaffected by the presence of the systems for which they are acting as reference frames. In some cases relatively uncontroversial examples exist, such as for the cartesian axes associated with the translation and rotation groups associated with the single particle system. The physical reference system may be a large magnet whose magnetic field points in a well defined direction and defines a z axis, combined with an electrostatic generator whose electric field is in another well defined direction at right angles that defines an x axis. In other cases the existence of suitable reference frames is less clear.

In this SubSection we will describe possible phase reference frames as if they are entirely separated (or uncorrelated) with the system of interest. In terms of the treatment by Bartlett et al [42], [31] these are non-implicated reference frames. In the next SubSection and in the next Appendix phase reference frames that are correlated with the system of interest will be described - these are the so-called implicated reference frames of Bartlett et al.

For the large quantum system with a well-defined reference phase associated with the \( U(1) \) group in the case of multi-mode or single mode systems involving identical particles, the usual choice is a single mode bosonic system such as a single mode \( \text{BEC} \) or a laser with a large mean occupancy, and which is thought of as being prepared in a Glauber coherent state \( |\Phi(\alpha)\rangle \) in order to provide the phase reference frame, the reference phase being \( \text{arg} \alpha \). Whether such a reference frame really exists is controversial. The discussion presented above in SubSections 2.10 and 2.12 raises the question of whether such a phase reference state could ever be prepared, so this choice of a physical phase reference is rather
unsatisfactory. However, from the point of view of this presentation we assume it does, so that - as in the previous example - Alice can describe the reference state as another coherent state. Again, whether Alice could ever prepare such a state is questionable.

Another possibility for a physical phase reference is a macroscopic low frequency harmonic oscillator, whose quantum energy eigenstates $|n\rangle$ - with $n = 0, 1, \ldots, n_{\text{max}}$ and energies $n\hbar\omega$ can be used to construct phase eigenstates $|\theta_p\rangle$ with $p = 0, 1, \ldots, n_{\text{max}}$ and $\theta_p = p \times 2\pi/(n_{\text{max}} + 1)$, and which are defined by

$$|\theta_p\rangle = \frac{1}{\sqrt{n_{\text{max}} + 1}} \sum_{n=0}^{n_{\text{max}}} \exp(in\theta_p) |n\rangle$$

(281)

These states are orthonormal. The separation between the equally spaced phase angles $\Delta \theta = 2\pi/(n_{\text{max}} + 1)$ can be made very small if $n_{\text{max}}$ is large enough. Under the effect of the harmonic oscillator Hamiltonian $\hat{H} = \hbar\omega \hat{N}$, where $\hat{N}$ is the number operator, the phase state $|\theta_p\rangle$ evolves into $|\theta_p - \omega\Delta t\rangle$ during a time interval $\Delta t$, so if the time intervals are chosen so that $\omega\Delta t = 2\pi/(n_{\text{max}} + 1)$, the phase angle $\theta_p$ changes into $\theta_{p-1}$. Thus the system behaves like a backwards running clock [58], the phase angles $\theta_p$ defining the positions of the hands. If the clock initially has phase $\theta_p$ the probability of finding the clock to have phase $\theta_q$ after a time interval $\Delta t$ is given by

$$P(\theta_q, \theta_p, \Delta t) = \frac{1}{(n_{\text{max}} + 1)^2} \frac{\sin^2((n_{\text{max}} + 1)\Delta/2)}{\sin^2(\Delta/2)}$$

(282)

where $\Delta = \theta_p - \theta_q - \omega\Delta t$. For times $\Delta t$ such that $\omega\Delta t \ll 2\pi/(n_{\text{max}} + 1)$ the probability of the phase remaining as $\theta_p$ is close to unity. Thus if the phase state $|\theta_p\rangle$ is used as a phase reference, it will remain stable for a time $\Delta t$ satisfying the last inequality. For $\Delta t \sim 100\mu s$ and $n_{\text{max}} \sim 10^4$ so that phase is defined to $\sim 10^{-3}$ radians, an oscillator frequency $\omega \sim 10^6$ s$^{-1}$ would suffice for this phase reference standard. Such macroscopic oscillators do exist, though the process to prepare them in the phase reference quantum state $|\theta_p\rangle$ would be technically difficult. Whether such a system would be useful as a phase reference for optical fields or a BEC is another issue.

12.7 Relational Description of Phase References

In this SubSection phase reference frames that are correlated with the system of interest will be described - these are the so-called implicate reference frames of Bartlett et al [52, 51].

One such approach to describing phase references in the $U(1)$ group case is via the concept of maps. For simplicity consider a one mode system $S$, the basis vectors for which are Fock states $|m\rangle_S$, where it is sufficient to restrict $m = 0, 1, \ldots, m_{\text{max}}$. The reference system $R$, will also be a one mode system with Fock states $|n\rangle_R$, where $n$ is large. Product states $|m\rangle_S \otimes |n\rangle_R$ for the combined modes exist in the Hilbert space $H_S \otimes H_R$ and are eigenstates of the
various number operators, including the total number operator $\hat{N}_T = \hat{N}_S + \hat{N}_R$ - where the eigenvalue is $l = m + n$. The product states may be listed via $m = 0, 1, \ldots, m_{\text{max}}$ and $n = 0, 1, \ldots, m_{\text{max}}$ and $l = m, m + 1, \ldots$. Here we will describe how a coherent superposition of number states, such as a Glauber coherent state can be represented.

In the so-called *internalisation* or *quantisation* of the reference frame the product state $|m\rangle_S \otimes |n\rangle_R$ is mapped onto the product state $|m\rangle_S \otimes |n - m\rangle_R$ where $n \geq m_{\text{max}}$. Thus

$$|m\rangle_S \otimes |n\rangle_R \rightarrow |m\rangle_S \otimes |n - m\rangle_R$$

(283)

Hence for a linear combination of system states given by

$$|\Phi\rangle_S = \sum_{m=0}^{m_{\text{max}}} C_m |m\rangle_S$$

we have for the state $|\Phi\rangle_S \otimes |n\rangle_R$ in $H_S \otimes H_R$

$$|\Phi\rangle_S \otimes |n\rangle_R = \sum_{m=0}^{m_{\text{max}}} C_m |m\rangle_S \otimes |n\rangle_R \rightarrow \sum_{m=0}^{m_{\text{max}}} C_m |m\rangle_S \otimes |n - m\rangle_R = |\Psi_{nRS}\rangle$$

(285)

The mapping results in an entangled state where there are $n$ bosons distributed between the two modes. This state $|\Psi_{nRS}\rangle$ is a pure state which is compatible with the SSR and is in one-one correspondence with the original system state $|\Phi\rangle_S$. Note that to create this state the reference state $|n\rangle_R$ must have more bosons in it than $m_{\text{max}}$. The density operator for the original pure system $S$ state would be $\hat{\sigma}_S = |\Phi\rangle_S \langle \Phi|_S$, and we note that this state violates the SSR. The state $|\Phi\rangle_S$ would be essentially a Glauber coherent state if $C_m = \exp(-|\alpha|^2/2)m^m/(\sqrt{m!})$, with $m_{\text{max}} \gg |\alpha|^2$. However, for the mapped state $|\Psi_{nRS}\rangle$ the reduced density operator $\hat{\rho}_S$ is given by

$$\hat{\rho}_S = \text{Tr}_R(|\Psi_{nRS}\rangle \langle \Psi_{RS}|)$$

$$= \sum_{m=0}^{m_{\text{max}}} |C_m|^2 |m\rangle_S \langle m|_S$$

(286)

This is a mixed state and is compatible with the SSR. For the Glauber coherent state $|\Phi\rangle_S$ this is the Poisson distribution of number states. Hence the original SSR violating superposition of number states for system $S$ is mapped onto a state in the combined system for which the reduced density operator is a statistical mixture and is consistent with the SSR. $\hat{\sigma}_S$ would correspond to Alice’s description of the state, $\hat{\rho}_S$ to Charlie’s.

In the alternative so-called *externalisation* of the reference frame the mapping is between product states, and is the reverse of the previous mapping. The product state $|m\rangle_S \otimes |n\rangle_R$ is mapped onto the product state $|m\rangle_S \otimes |m + n\rangle_R$ in the Hilbert space $H_S \otimes H_R$ where the former is spanned by vectors $|m\rangle_S$ and the latter by vectors $|m + n\rangle_R$, and where $n \geq m_{\text{max}}$. Thus

$$|m\rangle_S \otimes |n\rangle_R \rightarrow |m\rangle_S \otimes |m + n\rangle_R$$

(287)
The mapping of the $H_S \otimes H_R$ state $|\Psi_n\rangle_{RS}$ then is
\[
|\Psi_n\rangle_{RS} = \sum_{m=0}^{m_{\text{max}}} C_m |m\rangle_S \otimes |n-m\rangle_R \\
\rightarrow \sum_{m=0}^{m_{\text{max}}} C_m |m\rangle_S \otimes |n\rangle_R = \left(\sum_{m=0}^{m_{\text{max}}} C_m |m\rangle_S\right) \otimes |n\rangle_R = |\Xi_n\rangle_{RS}
\]

(288)

The mapping results in a non-entangled state which is incompatible with the SSR. The state in the subspace $H_S$ is a coherent superposition of number states, whilst that in $H_R$ is a Fock state. The reduced density operator in $H_S$ is $\hat{\sigma}^S$ given by
\[
\hat{\sigma}^S = \text{Tr}_R(|\Xi_n\rangle_{RS}\langle\Xi_n|_{RS}) \\
= \sum_{m=0}^{m_{\text{max}}} \sum_{k=0}^{m_{\text{max}}} C_m C_k^* |m\rangle_S \langle k|_S 
\]

(289)

which is the same as $\hat{\sigma} = |\Phi\rangle_S \langle\Phi|_S$ and involves coherences between different number states in contradiction to the SSR. Clearly this second mapping just reverses the first one.

Of these two treatments of phase reference frames, the internalisation version has a closer link to physics in that the pure state $|\Psi_n\rangle_{RS}$ can in principle be created and does lead to a way of creating a state that is in one-one correspondence with any SSR violating pure state $|\Phi\rangle_S$, though it is in the form of an entangled state of the $S, R$ sub-systems rather than just $S$ alone. This is an important point to note - the original SSR violating state does not exist as a state of a separate system, all that exists is an SSR compatible entangled state that is in one-one correspondence with it. However, the general process for creating a state such as $|\Psi_n\rangle_{RS}$ is not explained. For simple cases such as $|\Phi\rangle_S = (|0\rangle_S + |1\rangle_S)/\sqrt{2}$ the creation of the required state $|\Psi_n\rangle_{RS} = (|0\rangle_S \otimes |n\rangle_R + |1\rangle_S \otimes |n-1\rangle_R)/\sqrt{2}$, where $n \geq 1$ would seem feasible via the ejection of one boson from a BEC in a Fock state $|n\rangle_R$ into a previously unoccupied mode.

12.8 Irreducible Matrix Representations and Super-selection Rules

If $|i\rangle$ ($i = 1,2,..$) are a set of orthonormal basis vectors in the system state space, then the group of unitary operators $\hat{T}(g)$ is represented by a group of unitary matrices $D(g)$
\[
\hat{T}(g) |i\rangle = \sum_j D_{ji}(g) |j\rangle
\]

(290)

with elements $D_{ji}(g)$, and such that $D(hg) = D(h)D(g)$ etc corresponding to the group properties of the operators. This is a matrix representation of the transformation group.
The theory of such group representations and their application to quantum systems is well established, following the pioneering work of Wigner in the 1930s. We can just use the results here. A key concept is that of irreducible representations. Within the system state space we can in general choose so-called irreducible sub-spaces, denoted as $\Gamma_\alpha$ of dimension $d_\alpha$ and spanned by new orthonormal basis vectors $|\Gamma_\alpha \lambda\rangle$ ($\lambda = 1, 2, \ldots, d_\alpha$) such that

$$\hat{T}(g) |\Gamma_\alpha \lambda\rangle = \sum_{\mu=1}^{d_\alpha} D^\alpha_{\mu \lambda}(g) |\Gamma_\alpha \mu\rangle$$

(291)

For each irreducible sub-space $\Gamma_\alpha$ there is no smaller sub-space for which the operation of all $\hat{T}(g)$ just leads to linear combinations of vectors within that sub-space. The $d_\alpha \times d_\alpha$ matrices $D^\alpha(g)$ then form an irreducible matrix representation for the transformation group. For different $\alpha$ the representations are said to be inequivalent.

The irreducible matrices satisfy the so-called great orthogonality theorem [89]

$$\int w(g) dg D^\alpha_{\mu \lambda}(g) D^\beta_{\xi \tau}(g)^* = \frac{1}{d_\alpha} \delta_{\alpha \beta} \delta_{\mu \xi} \delta_{\lambda \tau}$$

(292)

The proof of this result is based on Schur’s lemma.

The importance of the irreducible representations and the consequent orthogonality theorem lies in its application to Situation B cases, where we have seen that Charlie’s density operator $\hat{\rho}$ is invariant under any of the transformations $\hat{T}(h) \hat{\rho} \hat{T}(h)^{-1} = \hat{\rho}$. Suppose we represent $\hat{\rho}$ in terms of the basis vectors $|\Gamma_\alpha \lambda\rangle$ associated with the irreducible representations

$$\hat{\rho} = \sum_{\alpha} \sum_{\lambda} \sum_{\beta \tau} R_{\alpha \beta \lambda \tau} |\Gamma_\alpha \lambda\rangle \langle \Gamma_\beta \tau|$$

(293)

where $R$ will be a Hermitian, positive definite matrix with unit trace since it represents a density operator. Applying the transformation gives

$$\hat{T}(h) \hat{\rho} \hat{T}(h)^{-1} = \sum_{\alpha \lambda \mu} \sum_{\beta \tau \xi} R_{\alpha \beta \lambda \tau} D^\alpha_{\mu \lambda}(h) |\Gamma_\alpha \mu\rangle \langle \Gamma_\beta \xi| D^\beta_{\xi \tau}(h)^*$$

(294)

Averaging over $h$ and using the great orthogonality theorem gives

$$\hat{\rho} = \sum_{\alpha} \sum_{\mu} \left( \sum_{\lambda} \frac{1}{d_\alpha} R^\alpha_{\lambda \lambda} \right) |\Gamma_\alpha \mu\rangle \langle \Gamma_\alpha \mu|$$

(295)

This is in the form of a mixed state involving irreducible state vectors $|\Gamma_\alpha \mu\rangle$ each occurring with a probability $P^\alpha_{\mu}$ given by

$$P^\alpha_{\mu} = \sum_{\lambda} \frac{1}{d_\alpha} R^\alpha_{\lambda \lambda} = P^\alpha$$

(296)
which is the same for all $\mu$ associated with a given irreducible representation $\Gamma_\alpha$. This is clearly a positive real quantity and since
\[
\sum_\alpha \sum_\mu P_\mu^\alpha = \sum_\alpha \sum_\mu \sum_\lambda \frac{1}{d_{\lambda\lambda}} R_{\lambda\lambda}^{\alpha\mu} = \sum_\alpha \sum_\lambda R_{\lambda\lambda}^{\alpha\alpha} = \text{Tr} \hat{\rho} = 1
\] (297)
the probabilities sum to unity as required.

The final result for Charlie’s density operator
\[
\hat{\rho} = \sum_\alpha \sum_\mu P_\mu^\alpha |\Gamma_\alpha \mu\rangle \langle \Gamma_\alpha \mu|
\] (298)
demonstrates the presence of a super-selection rule. In Charlie’s description of the quantum state there are no coherences between states $|\Gamma_\alpha \mu\rangle$ associated with differing irreducible representations of the transformation group. This represents the general form of the SSR for all transformation groups in Situation B cases.

As an example, consider the $U(1)$ group and the single mode bosonic system. Since the Fock states satisfy $\hat{T}(\theta_a) |n_a\rangle = \exp(i n_a \theta_a) |n_a\rangle$ they form the basis for the irreducible representations of the $U(1)$ group, the occupation number $n_a$ specifying the irreducible representation and the $1 \times 1$ matrices $\exp(i n_a \theta_a)$ being the unitary matrices. Hence Charlie will describe the quantum state as
\[
\hat{\rho} = \sum_{n_a} P(n_a) |n_a\rangle \langle n_a|
\] (299)
which is a statistical mixture of Fock states with no coherences between different Fock states. This result is of the same form as in Eq. (102) and is in accord with the SSR on boson number.

As another example, consider the $U(1)$ group and the multi-mode bosonic system. Here sums of products of Fock states
\[
|n_1 n_2 \ldots n_a; N\rangle = \prod_a |n_1\rangle \langle n_2| \ldots |n_a\rangle \ldots \quad N = \sum_a n_a
\] (300)
such that the total occupancy is $N = \sum_a n_a$ can be used to form irreducible representations for the transformation group in terms of linear combinations of the products with the same $N$. Writing these linear combinations as
\[
|\Psi^\mu_N\rangle = \sum_{\{n_1 n_2 \ldots n_a\}} C^N_{\{n_1 n_2 \ldots n_a\}} |n_1 n_2 \ldots n_a; N\rangle
\] (301)
we have since $\hat{T}(\theta) |n_1 n_2 \ldots n_a; N\rangle = \exp(i N \theta) |n_1 n_2 \ldots n_a; N\rangle$ we see that $\hat{T}(\theta) |\Psi^\mu_N\rangle = \exp(i N \theta) |\Psi^\mu_N\rangle$ also, so the $|\Psi^\mu_N\rangle$ define the irreducible basis states. The total occupancy $N$ specifies the irreducible representation, but here there
are many irreducible representations with the same \( N \) depending on the various \( \mu \). In this case Charlie will describe the state as

\[
\hat{\rho} = \sum_N \sum_\mu P^N_\mu |\Psi^\mu_N\rangle \langle \Psi^\mu_N|
\]  

(302)

which is a statistical mixture of multi-mode states \( |\Psi^\mu_N\rangle \) all with the same total occupancy \( N \). Although there are coherence terms between individual modal Fock states, there are no coherences between states with different total occupancy. This result is of the same form as in Eq. (83) and again is an example of a super-selection rule operating in terms of Charlie’s description of the quantum state.

Finally, we note that in situation A where the relationship between the frames is known and there is no invariance for Charlie’s density operator, we do not have SSR applying. For the single particle case and the translation group the momentum states \( |p\rangle \) define the irreducible representations, each specified by \( p \), and as we saw Charlie’s description of the quantum state involved linear combinations of these irreducible basis vectors, in contradiction to the SSR.

12.9 Non-Entangled States

The essential feature of an non-entangled or separable state is that the sub-systems are considered to be unrelated to each other. Hence, both for Alice and Charlie there will be separate reference frames for each sub-system, with transformation groups - \( \hat{T}_A(g_a) \) for sub-system A, \( \hat{T}_B(g_b) \) for sub-system B, etc which relate the reference systems of Alice to those of Charlie. The transformations \( g_a, g_b, .. \) are different. The overall transformation operator would be of the form \( \hat{T}(g_a,g_b,..) = \hat{T}_A(g_a) \otimes \hat{T}_B(g_b) \otimes .. \). Alice would describe a general non-entangled state as having a density operator

\[
\hat{\sigma} = \sum_R P^A_R \hat{\sigma}^A_R \otimes \hat{\sigma}^B_R \otimes \hat{\sigma}^C_R \otimes ...
\]  

(303)

It then follows for Situation B where the reference frames for Alice and Charlie are unrelated, that Charlie would describe the same state via the density operator

\[
\hat{\rho} = \sum_R P^A_R \hat{\rho}^A_R \otimes \hat{\rho}^B_R \otimes \hat{\rho}^C_R \otimes ...
\]  

(304)

where

\[
\hat{\rho}^C_R = \int w(g_c) dg_c \hat{T}_C(g_c) \hat{\sigma}^C_R \hat{T}_C^{-1}(g_c) \quad C = A, B,..
\]  

(305)

Note that separate twirl operations are applied to the different sub-systems, as explicitly shown in the papers by Vaccaro et al [34] (see Section IIIA, Eqn. 3.3 therein) and Paterek et al [36] (see Section 6). This leads for general transformation groups to the \textit{local group super-selection rule}, where the \( \hat{\rho}^C_R \) involve
no coherences between states associated with differing irreducible representations of the transformation group. We see that Charlie also describes a non-entangled state and with the same mixture probability $P_R$ as for Alice. Thus non-entanglement or separability is a feature that is the same for both Alice and Charlie, as ought to be the case.

In the context of sub-systems consisting of modes (or sets of modes) occupied by identical bosons, the case of interest is Situation B, with each transformation group being U(1). Here the relationship between Charlie’s and Alice’s phase reference frames are unknown. Hence irrespective of Alice’s description of the sub-system states $\sigma_R^A, \sigma_R^B, ...$ we see from the previous section that Charlie will describe the separate sub-system states $\rho_R^A, \rho_R^B$, as statistical mixtures of number states for the separate modes (or total number states for the sets of modes in each sub-system). Thus from Charlie’s point of view the separate mode density operators will satisfy the SSR. Thus we see that the introduction of reference frames and two observers - Charlie being the external one whose description of the quantum states is of primary interest - leads to the same SSR outcome as the simpler considerations set out in SubSections 2.10 and 2.12. Essentially the same considerations have been used in [25], [34] and the other papers to justify the local photon number superselection rule.
13 Appendix 5 - Super-Selection Rule Violations

13.1 Preparation of Coherent Superposition of an Atom and a Molecule

A key paper dealing with the coherent superposition of an atom and a molecule is that by Dowling et al [71], entitled “Observing a coherent superposition of an atom and a molecule”. Essentially the process involves one atom $A$ interacting with a BEC of different atoms $B$ leading to the creation of one molecule $AB$, with the BEC being depleted by one $B$ atom.

13.1.1 Hamiltonian

The Hamiltonian is given by

$$\hat{H} = \hbar \omega_A \hat{b}_A^\dagger \hat{b}_A + \hbar \omega_M \hat{b}_M^\dagger \hat{b}_M + \hbar \omega_2 \hat{b}_2^\dagger \hat{b}_2 + \frac{\hbar \kappa}{2} (\hat{b}_M^\dagger \hat{b}_A \hat{b}_2 + \hat{b}_M \hat{b}_A^\dagger \hat{b}_2^\dagger)$$  (306)

where $\hat{b}_A$, $\hat{b}_M$ and $\hat{b}_2$ are standard bosonic annihilation operators for the atom, molecule and BEC modes respectively, $\omega_A$, $\omega_M$ and $\omega_2$ are the corresponding mode frequencies and $\kappa$ defines the interaction strength for the process where a molecule is created or destroyed from/to an atom $A$ and a BEC atom $B$. $\Delta$ is the frequency difference between the molecular state $AB$ and the two separate states for atoms $A$ and $B$ – this is zero on Feshbach resonance - and is given by

$$\Delta = \omega_M - \omega_A - \omega_2$$  (307)

The Hamiltonian commutes with the total number operator $\hat{N}_{tot}$, where

$$\hat{N}_{tot} = 2 \hat{b}_M^\dagger \hat{b}_M + \hat{b}_A^\dagger \hat{b}_A + \hat{b}_2^\dagger \hat{b}_2$$  (308)

where the molecule number operator is multiplied by two.

13.1.2 Initial State

Initially the state of the system is given by the density operator Eqs (10) and (11) in the paper

$$\hat{W}_{0L} = \int \frac{d\theta}{2\pi} \exp(-i \hat{N}_{tot} \theta) |\Psi\rangle_{0L} \langle \Psi|_{0L} \exp(+i \hat{N}_{tot} \theta)$$  (309)

$$|\Psi\rangle_{0L} = |A\rangle |\beta\rangle$$  (310)

where $|A\rangle$ is a state with one atom $A$ and $|\beta\rangle$ is a Glauber coherent state for the BEC of atoms $B$. The super-operator acting on the pure state $|\Psi\rangle_{0L} \langle \Psi|_{0L}$ is called the *twirling operator*, the group of unitary operators $\exp(-i \hat{N}_{tot} \theta)$ depend on a phase variable $\theta$ and are a unitary representation of $U(1)$, the *generator*
being $\hat{N}_{tot}$. These operators act as a symmetry group for the system and leave the Hamiltonian invariant. The initial state is also given by

$$\hat{\rho}_A - M(0) = |A\rangle \langle A|$$

$$\hat{\rho}_2(0) = \int \frac{d\theta}{2\pi} |\beta\rangle \langle \beta| \exp(i\hat{n}_2\theta)$$

$$= \sum_n p_n <n|n\rangle$$

$$= \int \frac{d\theta}{2\pi} |\beta\rangle \langle \beta| \exp(-i\theta)$$

where $\hat{n}_2 = \hat{b}_2^\dagger \hat{b}_2$ is the number operator for the BEC mode and $p_n <n|n\rangle = \{\exp(-n/n!) <n|n\rangle /n!\}$ is a Poisson distribution, whose mean is $<n> = |\beta|^2$. Initially then there is one atom A and the BEC is in a statistical mixture of number states with a Poisson distribution, which is mathematically equivalent to a statistical mixture of Glauber coherent states $|\beta\rangle \langle \beta|$ with the same amplitude $\sqrt{<n>}$ but with all phases $(\arg \beta + \theta)$ being equally weighted.

### 13.1.3 Implicated Reference Frame

In the paper by Dowling et al [71] the BEC is acting as an implicated phase reference frame (see [42], [31]). The state of the reference frame as described by Charlie is given by

$$\hat{\rho}_{REF} = \hat{\rho}_2(0) = \int \frac{d\theta}{2\pi} |\beta\rangle \langle \beta| \exp(i\hat{n}_2\theta)$$

and from Eq. (306), there is an interaction between the reference BEC and the separate atom A and molecule M systems. However, because $<n> = |\beta|^2$ is very large, the BEC is essentially unchanged during the process, as reflected in the use of approximations in eqs (27), (28) of the paper. Another implicated phase reference frame situation, but involving a two mode reference frame is discussed in the paper by Paterek et al [36].

Overall, in terms of the discussion in Appendix 12 $\hat{W}_{0L}$ would be Charlie’s description of the initial state, whereas Alice would describe it as $|\Psi\rangle_{0L} \langle \Psi|_{0L}$. Presumably in the paper by Dowling et al [71] what is referred to as the “state of the laboratory” be Charlie’s reference frame, and what they refer to as the ”internal reference frame” would refer to that of Alice. However, whether Alice could actually prepare such a state as $|\Psi\rangle_{0L} \langle \Psi|_{0L}$ is controversial - see SubSections 2.10 and 2.12 though here this is assumed to be possible.

### 13.1.4 Process - Alice and Charlie Descriptions

There are three stages in the process, the first being with the interaction that turns separate atoms A and B into the molecule AB turned on at Feshbach.
resonance for a time \( t = \pi/(2\kappa < n >) \), the second being free evolution at large Feshbach detuning \( \Delta \) for a time \( \tau \) leading to a phase factor \( \phi = \Delta \tau \), the third being again with the interaction turned on at Feshbach resonance for a further time \( t = \pi/(2\kappa < n >) \). The typical initial state \( |\Psi\rangle_{0L} \) given by \(|A\rangle |\beta\rangle \) (eq (11)) evolves into \( |\Psi\rangle_{3L} \) given by (see eq. (32) of paper)

\[
|\Psi\rangle_{3L} = \left( \sin\left(\frac{\phi}{2}\right) |A\rangle - \exp(i \arg \beta) \cos\left(\frac{\phi}{2}\right) |M\rangle \right) |\beta\rangle
\]

using approximations set out in eqs (27), (28) of the paper that depend on \( < n > \) being large. Here \( |M\rangle \) is a state with one molecule AB. Thus it looks like a coherent superposition of an atom state \(|A\rangle\) and a molecule state \(|M\rangle\) has been prepared, the atom plus molecule system being disentangled from the BEC. *Alice* would describe the final state of the system as \( |\Psi\rangle_{3L} \langle \Psi|_{3L} \), so from her point of view a coherent superposition of an atom and a molecule has been prepared.

However, for *Charlie* the final state of the system is described by a density operator \( \hat{W}_{3L} \) which is reconstructed by applying the twirling operator to \( |\Psi\rangle_{3L} \langle \Psi|_{3L} \). Noting that

\[
\exp(-i \tilde{N}_{tot} \theta) |\Psi\rangle_{3L} = \left( \exp(-i \theta) \sin\left(\frac{\phi}{2}\right) |A\rangle - \exp(-2i \theta) \exp(i \arg \beta) \cos\left(\frac{\phi}{2}\right) |M\rangle \right) |\beta\rangle 
\]

and using

\[
Tr_2(|\beta\rangle \langle \beta| \exp(-i \theta)) = \langle \beta \exp(-i \theta) | \beta \exp(-i \theta) \rangle = 1 \quad (319)
\]

we see that Charlie’s final reduced density operator for the atom-molecule system is

\[
\hat{\rho}_{A-M}(3) = Tr_2 \hat{W}_{3L} \]

\[
= Tr_2 \int \frac{d\theta}{2\pi} \exp(-i \tilde{N}_{tot} \theta) |\Psi\rangle_{3L} \langle \Psi|_{3L} \exp(+i \tilde{N}_{tot} \theta) \]

\[
\int \frac{d\theta}{2\pi} \left( \exp(-i \theta) \sin\left(\frac{\phi}{2}\right) |A\rangle - \exp(-2i \theta) \exp(i \arg \beta) \cos\left(\frac{\phi}{2}\right) |M\rangle \right) \]

\[
\times \left( \exp(+i \theta) \sin\left(\frac{\phi}{2}\right) \langle A| - \exp(+2i \theta) \exp(-i \arg \beta) \cos\left(\frac{\phi}{2}\right) \langle M| \right)
\]

\[
= \sin^2\left(\frac{\phi}{2}\right) |A\rangle \langle A| + \cos^2\left(\frac{\phi}{2}\right) |M\rangle \langle M| \quad (320)
\]

Thus the coherence terms like \(|A\rangle \langle M|\) and \(|M\rangle \langle A|\) do not appear in the final density operator when the average over \( \theta \) (not \( \beta \)) is carried out.

For Charlie the density operator for the atom and molecule is of course a statistical mixture of a state with one atom and no molecule and a state with no atom and one molecule. The authors of [71] actually point this out in the paragraph after eq (35) where (presumably for the case \( \phi = \pi/4 \)) it is stated “the
state is found to be . . . an incoherent mixture of an atom and a molecule.”. The probabilities for detecting an atom A or a molecule AB are as in eq (33) of the paper. In terms of Charlie’s description, the density operator at the end of the preparation process does not signify the existence of a coherent superposition of an atom and a molecule, as the title to the paper might be taken to imply. The existence of such a coherent superposition would of course be present in Alice’s description, but it is Charlie’s (laboratory) description that is more relevant.

13.1.5 Coherence Effects Without SSR Violation

Note that coherence effects are still present since the atom or molecule detection probabilities depend on the phase $\phi$ associated with the free evolution stage of the process. However, as in many other instances, the presence of coherence effects does not require the existence of coherent superposition states that violate the super-selection rule. The authors actually point this out in the paragraph after eq (35), where it is stated “we have clearly predicted the standard operational signature of coherence, namely Ramsey type fringes, but the coherence is not present in our mathematical description of the system.” What they are referring to is Charlie’s description of the final state - which indeed shows no such coherence, but the belief that coherent superposition states are needed to predict coherence effects is mistaken.

To drive this point home, the process can be treated with the initial state for the BEC being given as a Fock state $|N\rangle$. With the interaction being given as in Eq.(306) (eq (14) in the paper) the state vector is a simple linear combination of two terms

$$|\Psi(t)\rangle = A(t) |A\rangle |N\rangle + B(t) |M\rangle |N-1\rangle$$  \hspace{1cm} (321)

This is of course an entangled state. Coupled equations for the two amplitudes $A(t)$ and $B(t)$ can easily be obtained and simple solutions obtained for stages where the Feshbach detuning is either zero or large. The state vector is continuous from one stage to the next, and the reduced density operator at the end of the three stage process for the atom plus molecule sub-system can be obtained. It is of the form

$$\hat{\rho}_{A-M}(3) = Tr_2(|\Psi(3)\rangle \langle \Psi(3)|)$$

$$= \sin^2(\frac{\phi}{2}) |A\rangle \langle A| + \cos^2(\frac{\phi}{2}) |M\rangle \langle M|$$  \hspace{1cm} (322)

which is of course a statistical mixture of a state with one atom and no molecule and a state with no atom and one molecule - and is exactly the same result as obtained in the paper by Dowling et al.\[71\]. Note that coherence effects in regard to the interferometric dependence on $\phi$ for measurements on the final state has been found without invoking either the description of the BEC via Glauber coherent states or the presence of a coherent superposition of an atomic and a molecular state. The result can easily be extended for the case where the BEC is initially in a statistical mixture of Fock states with differing $N$ occurring with
a probability \( P_N \). Each initial state \( |A\rangle |N\rangle \) evolves as in Eq. (321). We then would have

\[
\hat{\rho}_{A-M}(3) = Tr_2 \left( \sum_N P_N |\Psi_N(3)\rangle \langle \Psi_N(3)| \right)
\]

\[
= \sum_N P_N \left( \sin^2 \left( \frac{\phi}{2} \right) |A\rangle \langle A| + \cos^2 \left( \frac{\phi}{2} \right) |M\rangle \langle M| \right)
\]

which is the same as before. Allowing for a statistical mixture of Fock states makes no difference to the interferometric result.

13.1.6 Conclusion

Dowling et al [71] state in their abstract that “we demonstrate that it is possible to perform a Ramsey-type interference experiment to exhibit a coherent superposition of a single atom and a diatomic molecule”. However the interferometric or coherence effects (involving the dependence on \( \phi \)) cannot be said to exhibit the existence of such a coherent superposition, since the same interferometric results can be obtained without ever introducing such a quantum state. There is not a convincing case that quantum states that violate the super-selection rule forbidding the creation of coherent superpositions of Fock states with differing particle numbers can be created, even in Alice’s reference system. The fact that an SSR violating state \( |\Psi\rangle_3 \langle \Psi|_3 \) is created in Alice’s reference system is not surprising, because in the process considered the initial state \( |\beta\rangle \) for the BEC was assumed as a factor in Alice’s initial state, and this was itself inconsistent with the SSR. Furthermore, such SSR violating states are not needed to describe coherence and interference effects, so that justification for their physical existence also fails.

13.2 Detection of Coherent Superposition of a Vacuum and a One-Boson State ?

Whether such super-selection rule violating states can be detected has also not been justified. For example, consider the state given by a superposition of a one boson state and the vacuum state (as discussed in [72]). Consider an interferometric process in which one mode \( A \) for a two mode BEC interferometer is initially in the state \( \alpha |0\rangle + \beta |1\rangle \), and the other mode \( B \) is initially in the state \( |0\rangle \) - thus \( |\Psi(i)\rangle = (\alpha |0\rangle + \beta |1\rangle)_A \otimes |0\rangle_B \) in the usual occupancy number notation, where \( |\alpha|^2 + |\beta|^2 = 1 \). Modes \( A, B \) could refer to two different hyperfine states of a bosonic atom with non-relativistic energies \( \hbar \omega_A \) and \( \hbar \omega_B \), mode annihilation operators \( \hat{a}, \hat{b} \). The modes are first coupled by a beam splitter, which could be a resonant microwave pulse that causes transitions between the two hyperfine
states and which can be described via a unitary operator $\hat{U}_{BS}$ such that

$$
\hat{U}_{BS}(|1\rangle_A \otimes |0\rangle_B) = (|1\rangle_A \otimes |0\rangle_B - i |0\rangle_A \otimes |1\rangle_B) / \sqrt{2}
$$

$$
\hat{U}_{BS}(|0\rangle_A \otimes |1\rangle_B) = (-i |1\rangle_A \otimes |0\rangle_B + |0\rangle_A \otimes |1\rangle_B) / \sqrt{2}
$$

$$
\hat{U}_{BS}(|0\rangle_A \otimes |0\rangle_B) = (|0\rangle_A \otimes |0\rangle_B).
$$

(324)

After passing through the beam splitter the system is allowed to evolve freely for a time $\tau$, the Hamiltonian being

$$
\hat{H}_{\text{free}} = \left( \frac{mc^2}{\hbar} + \omega_A \right) \hat{a}^\dagger \hat{a} + \left( \frac{mc^2}{\hbar} + \omega_B \right) \hat{b}^\dagger \hat{b}
$$

where collisional effects have been ignored and the rest mass energy included for completeness. Following the free evolution stage, the modes are then coupled again via a beam splitter, and the probability of an atom being found in modes $A, B$ then being measured. A straightforward treatment of the evolution shows that the final state is given by

$$
|\Psi(f)\rangle = \alpha(|0\rangle_A \otimes |0\rangle_B) + \beta \exp(-i\{mc^2/\hbar + \omega_A\}\tau)
$$

$$
\times \left( \frac{1 - \exp(-i\Delta\tau)}{2} (|1\rangle_A \otimes |0\rangle_B) - i \frac{1 + \exp(-i\Delta\tau)}{2} (|0\rangle_A \otimes |1\rangle_B) \right)
$$

(325)

where $\Delta = \omega_B - \omega_A$ is the detuning. The probabilities of finding one atom in modes $A, B$ respectively are

$$
P_{10} = |\beta|^2 \sin^2(\Delta\tau/2) \quad P_{01} = |\beta|^2 \cos^2(\Delta\tau/2)
$$

(326)

Thus whilst coherence effects occur depending on the phase difference $\phi = \Delta\tau$ associated with the interferometric process, the overall detection probabilities only depend on the initial state via $|\beta|^2$. There is no dependence on the relative phase between $\alpha$ and $\beta$, as would be required if the superposition state $\alpha |0\rangle + \beta |1\rangle$ is to be specified from the measurement results. Exactly the same detection probabilities are obtained if the initial state is the mixed state

$$
\hat{\rho}(i) = |\alpha|^2 (|0\rangle_A \langle 0|_A \otimes |0\rangle_B) + |\beta|^2 (|1\rangle_A \langle 1|_A \otimes |0\rangle_B)
$$

in which the vacuum state for mode $A$ occurs with a probability $|\alpha|^2$ and the one boson state for mode $A$ occurs with a probability $|\beta|^2$. In this example the coherent superposition associated with the super-selection rule violating state would not be detected in the interferometric process. The paper by Dunningham et al [72] considers first a detection process that involves using a Glauber coherent state as one of the input states. Similar interference effects as in Eq. (326) are obtained. A second detection process in which the single term Glauber coherent state is replaced by a statistical mixture with all phases equally weighted in considered next, leading to the same interference effects. This again confirms that it is not necessary to invoke the existence of coherent superpositions of number states in order to demonstrate interference effects.
14 Appendix 6 - Non-Physical Two Mode States

We now consider some possible states for the second mode $B$ - to be combined with $\hat{\rho}_1^A$, $\hat{\rho}_2^A$ and $P_1$, $P_2$ as in Eq. (98). These states are two general pure orthogonal states of the form $\alpha |0\rangle_B + \beta |1\rangle_B$ and $-\beta^* |0\rangle_B + \alpha^* |1\rangle_B$ with $(|\alpha|^2 + |\beta|^2) = 1$. We have

\[
\begin{align*}
\hat{\rho}_1^B &= ((\alpha |0\rangle_B + \beta |1\rangle_B)) ((\alpha^* \langle 0|_B + \beta^* \langle 1|_B)) \\
\hat{\rho}_2^B &= ((-\beta |0\rangle_B + \alpha |1\rangle_B)) ((-\beta^* \langle 0|_B + \alpha^* \langle 1|_B))
\end{align*}
\]
(327)

This gives the reduced density operator

\[
\hat{\rho}_B = \frac{1}{2} (|0\rangle_B \langle 0|_B) + \frac{1}{2} (|1\rangle_B \langle 1|_B)
\]
(328)

A straightforward calculation gives for the overall density operator for the two mode non-entangled state as in Eq. (2)

\[
\hat{\rho} = \hat{\rho}_1 + \hat{\rho}_2
\]

where the $\hat{\rho}_1$, $\hat{\rho}_2$ are contributions that are consistent with or inconsistent with the super-selection rule. We have

\[
\hat{\rho}_1 = \frac{1}{4} |0\rangle_A \langle 0|_A \otimes |0\rangle_B \langle 0|_B + \frac{1}{4} |1\rangle_A \langle 1|_A \otimes |0\rangle_B \langle 0|_B + \frac{1}{4} |0\rangle_A \langle 0|_A \otimes |1\rangle_B \langle 1|_B + \frac{1}{4} |1\rangle_A \langle 1|_A \otimes |1\rangle_B \langle 1|_B
\]
\[
+ \frac{1}{2} \alpha^* \beta |0\rangle_A \langle 1|_A \otimes |1\rangle_B \langle 0|_B + \frac{1}{2} \alpha \beta^* |1\rangle_A \langle 0|_A \otimes |0\rangle_B \langle 1|_B
\]
(329)

and

\[
\hat{\rho}_2 = \frac{1}{4} (|\alpha|^2 - |\beta|^2) |0\rangle_A \langle 0|_A \otimes |0\rangle_B \langle 0|_B + \frac{1}{4} (|\alpha|^2 - |\beta|^2) |1\rangle_A \langle 0|_A \otimes |0\rangle_B \langle 0|_B + \frac{1}{4} (|\beta|^2 - |\alpha|^2) |0\rangle_A \langle 0|_A \otimes |1\rangle_B \langle 1|_B + \frac{1}{4} (|\beta|^2 - |\alpha|^2) |1\rangle_A \langle 1|_A \otimes |0\rangle_B \langle 1|_B
\]
\[
+ \frac{1}{2} \alpha^* \beta |1\rangle_A \langle 0|_A \otimes |1\rangle_B \langle 0|_B + \frac{1}{2} \alpha \beta^* |0\rangle_A \langle 1|_A \otimes |0\rangle_B \langle 1|_B
\]
(330)

Now to make $\hat{\rho}_2 = 0$ requires $|\alpha|^2 = |\beta|^2$ so that the first four terms in $\hat{\rho}_2$ are zero. This in combination with $|\alpha|^2 + |\beta|^2 = 1$ leads to $|\alpha| = |\beta| = \frac{1}{\sqrt{2}}$. However this results in the remaining two terms in $\hat{\rho}_2$ - which are coherences between $N = 0$ and $N = 2$ states - always being non-zero. Overall then, no choice of $\alpha$, $\beta$ will lead to an overall density operator which is physical. Adding further states $|2\rangle_B$, $|3\rangle_B$, ...does not rectify the problem.
15 Appendix 7 - Derivation of Sorensen et al Results

Sorensen et al [45] derive a number of inequalities from which they deduce a further inequality for the spin squeezing parameter in the case of a non-entangled state. From this result they conclude that spin squeezing implies entanglement.

The final inequality they obtain for a non-entangled state is

\[ \langle \Delta S_z^2 \rangle \geq \frac{1}{N} \left( \langle \hat{S}_z \rangle^2 + \langle \hat{S}_y \rangle^2 \right) \] (331)

Their approach is based on writing the density operator for a non-entangled state of identical particles as in Eq. (75),

\[ \hat{\rho} = \sum_R P_R \hat{\rho}_R \otimes \hat{\rho}_R \otimes \ldots = \sum_R P_R \hat{\rho}_R \] (332)

The spin operators are defined as \( \hat{S}_x = \sum_i \hat{S}_x^i = \sum_i (|\phi_b(i)\rangle \langle \phi_a(i)| + |\phi_a(i)\rangle \langle \phi_b(i)|)/2 \)

\[ \hat{S}_y = \sum_i \hat{S}_y^i = \sum_i (|\phi_b(i)\rangle \langle \phi_a(i)| - |\phi_a(i)\rangle \langle \phi_b(i)|)/2 \]

\[ \hat{S}_z = \sum_i \hat{S}_z^i = \sum_i (|\phi_b(i)\rangle \langle \phi_b(i)| - |\phi_a(i)\rangle \langle \phi_a(i)|)/2 \], where the sum \( i \) is over the identical atoms and each atom is associated with two states \( |\phi_a\rangle \) and \( |\phi_b\rangle \). Clearly, the spin operators satisfy the standard commutation rules for angular momentum operators.

Sorensen et al [45] state that the variance for \( \hat{S}_z \) satisfies the result

\[ \langle \Delta \hat{S}_z^2 \rangle = \frac{N}{4} - \sum_R P_R \sum_i \langle \hat{S}_z^i \rangle^2_R + \sum_R P_R \langle \hat{S}_z \rangle^2_R - \langle \hat{S}_z \rangle^2 \] (333)

To prove this we have

\[ \langle \hat{S}_z^2 \rangle = \sum_R P_R \text{Tr}(\hat{\rho}_R \sum_i \sum_j \hat{S}_z^i \hat{S}_z^j) \]

\[ = \sum_R P_R \left( \sum_i \langle \hat{S}_z^i \rangle^2_R + \sum_{i \neq j} \langle \hat{S}_z^i \rangle_R \langle \hat{S}_z^j \rangle_R \right) \]

\[ = \frac{N}{4} + \sum_R P_R \left( \sum_{i \neq j} \langle \hat{S}_z^i \rangle_R \langle \hat{S}_z^j \rangle_R \right) \] (334)

where we have used

\[ \langle \hat{S}_z^i \rangle^2 = \frac{1}{4} (|\phi_b(i)\rangle \langle \phi_b(i)| - |\phi_a(i)\rangle \langle \phi_a(i)|)^2 \]

\[ = \frac{1}{4} (|\phi_b(i)\rangle \langle \phi_b(i)| |\phi_b(i)\rangle \langle \phi_b(i)| - (|\phi_b(i)\rangle \langle \phi_b(i)| |\phi_a(i)\rangle \langle \phi_a(i)|) + (|\phi_a(i)\rangle \langle \phi_a(i)| |\phi_a(i)\rangle \langle \phi_a(i)|) \]

\[ + \frac{1}{4} (|\phi_a(i)\rangle \langle \phi_a(i)| |\phi_b(i)\rangle \langle \phi_b(i)|) + (|\phi_a(i)\rangle \langle \phi_a(i)| |\phi_a(i)\rangle \langle \phi_a(i)|) \]

\[ = \frac{1}{4} (|\phi_a(i)\rangle \langle \phi_b(i)| + |\phi_b(i)\rangle \langle \phi_a(i)| , \quad \frac{1}{4} S_{1i} \] (335)
a result based on the orthogonality, normalisation and completeness of the states $|\phi_a(i)\rangle, |\phi_b(i)\rangle$. Also

\[
\langle \hat{S}_z \rangle_R = \text{Tr}(\hat{\rho}_R \sum_i \hat{S}_z^i)
\]

\[
= \sum_i \langle \hat{S}_z^i \rangle_R
\]

\[
\sum_R P_R \langle \hat{S}_z \rangle_R^2 = \sum_R P_R \left( \sum_i \langle \hat{S}_z^i \rangle_R^2 + \sum_{i \neq j} \langle \hat{S}_z^i \rangle_R \langle \hat{S}_z^j \rangle_R \right)
\]  (336)

so eliminating the term $\sum_R P_R \left( \sum_{i \neq j} \langle \hat{S}_z^i \rangle_R \langle \hat{S}_z^j \rangle_R \right)$ gives the required expression for $\langle \Delta \hat{S}_z^2 \rangle = \langle \hat{S}_z^2 \rangle - \langle \hat{S}_z \rangle^2$.

Next, Sorensen et al. [45] state that

\[
\langle \hat{S}_x \rangle^2 \leq N \sum_R P_R \sum_i \langle \hat{S}_x^i \rangle_R^2
\]

\[
\langle \hat{S}_y \rangle^2 \leq N \sum_R P_R \sum_i \langle \hat{S}_y^i \rangle_R^2
\]  (337)

To prove this we have

\[
\langle \hat{S}_x \rangle = \sum_R P_R \text{Tr}(\hat{\rho}_R \sum_i \hat{S}_x^i)
\]

\[
= \sum_R P_R \sum_i \langle \hat{S}_x^i \rangle_R
\]

\[
| \langle \hat{S}_x \rangle | \leq \sum_R P_R \sum_i | \langle \hat{S}_x^i \rangle_R |
\]  (338)

since the modulus of a sum is less than or equal to the sum of the moduli. Now

\[
\langle \hat{S}_x \rangle^2 = | \langle \hat{S}_x \rangle |^2 \leq \left( \sum_R P_R \sum_i | \langle \hat{S}_x^i \rangle_R | \right)^2
\]

\[
\leq \sum_R P_R \left( \sum_i | \langle \hat{S}_x^i \rangle_R | \right)^2
\]  (339)

using the general result that $\left( \sum_R P_R \sqrt{C_R} \right)^2 \leq \sum_R P_R C_R$, where $\sum_R P_R = 1$ with here $\sqrt{C_R} = \sum_i | \langle \hat{S}_x^i \rangle_R |$. Next consider

\[
y = N \sum_i | \langle \hat{S}_x^i \rangle_R |^2
\]

\[
z = \left( \sum_i | \langle \hat{S}_x^i \rangle_R | \right)^2 = \left( \sum_i | \langle \hat{S}_x^i \rangle_R | \right)^2
\]

\[
y - z = \sum_{i < j} (| \langle \hat{S}_x^i \rangle_R | - | \langle \hat{S}_x^j \rangle_R |)^2 \geq 0
\]  (340)
so that
\[
\langle \hat{S}_x \rangle^2 \leq N \sum_R P_R \sum_i |\langle \hat{S}_x^i \rangle_R |^2 \quad \langle \hat{S}_y \rangle^2 \leq N \sum_R P_R \sum_i |\langle \hat{S}_y^i \rangle_R |^2
\] (341)

which is the required result. The inequality for \( \langle \hat{S}_y \rangle^2 \) is proved similarly.

Another inequality is stated [45] for \( \langle \hat{S}_z \rangle^2 \). This is
\[
\langle \hat{S}_z \rangle^2 \leq \sum_R P_R \langle \hat{S}_z \rangle_R^2
\] (342)

To show this we have
\[
\langle \hat{S}_z \rangle = \sum_R P_R Tr(\hat{\rho}_R \sum_i \hat{S}_z^i)
\]
\[
= \sum_R P_R \sum_i \langle \hat{S}_z^i \rangle_R
\]
\[
= \sum_R P_R \langle \hat{S}_z \rangle_R
\]
\[
|\langle \hat{S}_z \rangle| \leq \sum_R P_R |\langle \hat{S}_z \rangle_R |
\] (343)

so that
\[
\langle \hat{S}_z \rangle^2 = |\langle \hat{S}_z \rangle|^2 \leq \left( \sum_R P_R |\langle \hat{S}_z \rangle_R | \right)^2
\]
\[
\leq \sum_R P_R |\langle \hat{S}_z \rangle_R |^2
\]
\[
= \sum_R P_R \langle \hat{S}_z \rangle_R^2
\] (344)

using the general result that \( \left( \sum_R P_R \sqrt{C_R} \right)^2 \leq \sum_R P_R C_R \), where \( \sum_R P_R = 1 \) with

here \( \sqrt{C_R} = |\langle \hat{S}_z \rangle_R | \).

Finally, we find that
\[
\sum_R P_R \sum_i \left( \langle \hat{S}_x^i \rangle_R^2 + \langle \hat{S}_y^i \rangle_R^2 + \langle \hat{S}_z^i \rangle_R^2 \right) \leq \frac{1}{4} N
\]
\[
- \sum_R P_R \sum_i \langle \hat{S}_z^i \rangle_R^2 \geq -\frac{1}{4} N + \sum_R P_R \sum_i \left( \langle \hat{S}_x^i \rangle_R^2 + \langle \hat{S}_y^i \rangle_R^2 \right)
\] (345)
To show this we use the properties of the density operator $\hat{\rho}_R$ for the $i$th particle of Hermitiancy, positiveness, unit trace $Tr(\hat{\rho}_R^\dagger) = 1$ and $Tr(\hat{\rho}_R^2) \leq 1$. In terms of matrix elements of the density operator $\hat{\rho}_R$ between the two states $|\phi_a(i)\rangle$, $|\phi_b(i)\rangle$ the quantities $\langle \hat{S}_x^i \rangle_R$, $\langle \hat{S}_y^i \rangle_R$ and $\langle \hat{S}_z^i \rangle_R$ are

$$
\begin{align*}
\langle \hat{S}_x^i \rangle_R &= Tr(\hat{\rho}_R^\dagger \frac{1}{2} (|\phi_b(i)\rangle \langle \phi_a(i)| + |\phi_a(i)\rangle \langle \phi_b(i)|)) \\
&= \frac{1}{2} (\rho^i_{ab} + \rho^i_{ba}) \\
\langle \hat{S}_y^i \rangle_R &= \frac{1}{2i} (\rho^i_{ab} - \rho^i_{ba}) \\
\langle \hat{S}_z^i \rangle_R &= \frac{1}{2} (\rho^i_{bb} - \rho^i_{aa})
\end{align*}
$$

where $\rho^i_{cd} = \langle \phi_c(i)|\hat{\rho}_R^\dagger|\phi_d(i)\rangle$. The Hermitiancy and positiveness of $\hat{\rho}_R$ show that $\rho^i_{bb}$ and $\rho^i_{aa}$ are real and positive, $\rho^i_{ab} = (\rho^i_{ba})^*$ and $\rho^i_{aa} \rho^i_{bb} - |\rho^i_{ab}|^2 \geq 0$. The condition $Tr(\hat{\rho}_R^2) = 1$ leads to $\rho^i_{aa} + \rho^i_{bb} = 1$, from which $Tr(\hat{\rho}_R^2) \leq 1$ follows using the previous positivity results. Taken together these conditions lead to the following useful parametrisation of the density matrix elements

$$
\begin{align*}
\rho^i_{aa} &= \sin^2 \alpha_i, \quad \rho^i_{bb} = \cos^2 \alpha_i \\
\rho^i_{ab} &= \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i \sin^2 \beta_i \exp(+i \phi_i)}, \quad \rho^i_{ba} = \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i \sin^2 \beta_i \exp(-i \phi_i)}
\end{align*}
$$

where $\alpha_i$, $\beta_i$ and $\phi_i$ are real. In terms of these quantities we then have

$$
\begin{align*}
\langle \hat{S}_x^i \rangle_R &= \frac{1}{2} \sin 2\alpha_i \sin^2 \beta_i \cos \phi_i \\
\langle \hat{S}_y^i \rangle_R &= \frac{1}{2} \sin 2\alpha_i \sin^2 \beta_i \sin \phi_i \\
\langle \hat{S}_z^i \rangle_R &= \frac{1}{2} \cos 2\alpha_i
\end{align*}
$$

It is then easy to show that

$$
\langle \hat{S}_x^i \rangle_R^2 + \langle \hat{S}_y^i \rangle_R^2 + \langle \hat{S}_z^i \rangle_R^2 = \frac{1}{4} - \frac{1}{4} \sin^2 2\alpha_i (1 - \sin^4 \beta_i) \leq \frac{1}{4}
$$

and the final inequality (345) then follows by taking the sum over particles $i$ and then using $\sum_i P_R = 1$. If only the Schwarz inequality is used instead of the more detailed consequences of Hermitiancy, positiveness etc it can be shown that $\langle \hat{S}_x^i \rangle_R^2 + \langle \hat{S}_y^i \rangle_R^2 + \langle \hat{S}_z^i \rangle_R^2 \leq \frac{4}{9}$, which though correct is not useful.

Combining the inequalities in Eqs. (337), (341) and (345) into Eq. (333)
shows that

\[
\langle \Delta \hat{S}_z^2 \rangle = \frac{N}{4} - \sum_R P_R \sum_i \langle \hat{S}_z^i \rangle_R^2 + \sum_R P_R \langle \hat{S}_z \rangle_R^2 - \langle \hat{S}_z \rangle^2
\]

\[
\geq \frac{N}{4} - \sum_R P_R \sum_i \langle \hat{S}_z^i \rangle_R^2
\]

\[
\geq \frac{N}{4} - \frac{1}{4} N + \sum_R P_R \sum_i \left( \langle \hat{S}_x^i \rangle_R^2 + \langle \hat{S}_y^i \rangle_R^2 \right)
\]

\[
\geq \frac{1}{N} \left( \langle \hat{S}_x \rangle^2 + \langle \hat{S}_y \rangle^2 \right)
\]

(350)

for the case of a non-entangled state. This result is that in Sorensen et al. [45].
16 Appendix 8 - Revised Sorensen et al

16.1 Variance $\langle \Delta \hat{S}_x^2 \rangle$

Here we will see if the modified approach to Sorensen et al can lead to a useful inequality for $\langle \Delta \hat{S}_x^2 \rangle$ or $\langle \Delta \hat{S}_y^2 \rangle$ that applies when non-entangled states are those when all the separate modes $\hat{a}_i$ and $\hat{b}_i$ are the sub-systems. We will attempt to follow the approach used for the simple two mode case in Section 4.

Firstly, the variance for a Hermitian operator $\hat{\Omega}$ in a mixed state

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R$$

is always greater than or equal to the average of the variances for the separate components

$$\langle \Delta \hat{\Omega}^2 \rangle \geq \sum_R P_R \langle \Delta \hat{\Omega}^2 \rangle_R$$

where $\langle \Delta \hat{\Omega}^2 \rangle = Tr(\hat{\rho} \Delta \hat{\Omega}^2)$ with $\Delta \hat{\Omega} = \hat{\Omega} - \langle \hat{\Omega} \rangle$ and $\langle \Delta \hat{\Omega}^2 \rangle_R = Tr(\hat{\rho}_R \Delta \hat{\Omega}_R^2)$ with $\Delta \hat{\Omega}_R = \hat{\Omega} - \langle \hat{\Omega} \rangle_R$. The proof is straight-forward and given in Ref. [78].

Next we calculate $\langle \Delta \hat{S}_x^2 \rangle_R$, $\langle \Delta \hat{S}_y^2 \rangle_R$ and $\langle \hat{S}_x \rangle_R$, $\langle \hat{S}_y \rangle_R$, $\langle \hat{S}_z \rangle_R$ for the case where

$$\hat{\rho} = \sum_R P_R (\hat{\rho}_R^a \otimes \hat{\rho}_R^b) \otimes (\hat{\rho}_R^2 \otimes \hat{\rho}_R^2) \otimes (\hat{\rho}_R^3 \otimes \hat{\rho}_R^3).$$

as is required for a general non-entangled state all $2N$ modes. Furthermore, the density operators for the individual modes must represent possible physical states for such modes, so the super-selection rule for atom number applies and we have

$$\langle (\hat{a}_i)^n \rangle_{a_i} = Tr(\hat{\rho}_R^a (\hat{a}_i)^n) = 0 \quad \langle (\hat{a}_i)^n \rangle_{a_i} = Tr(\hat{\rho}_R^a (\hat{a}_i)^n) = 0$$

$$\langle (\hat{b}_i)^m \rangle_{b_i} = Tr(\hat{\rho}_R^b (\hat{b}_i)^m) = 0 \quad \langle (\hat{b}_i)^m \rangle_{b_i} = Tr(\hat{\rho}_R^b (\hat{b}_i)^m) = 0$$

(354)

The Schwinger spin operators are

$$\hat{S}_x = \sum_i (\hat{b}_i^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{b}_i)/2 = \sum_i \hat{S}_x^i$$

$$\hat{S}_y = \sum_i (\hat{b}_i^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{b}_i)/2i = \sum_i \hat{S}_y^i$$

$$\hat{S}_z = \sum_i (\hat{b}_i^\dagger \hat{b}_i - \hat{a}_i^\dagger \hat{a}_i)/2 = \sum_i \hat{S}_z^i$$

(355)
where \( \hat{a}_i, \hat{b}_i \) and \( \hat{a}_i^\dagger, \hat{b}_i^\dagger \) respectively are mode annihilation, creation operators.

From Eqs. (355) we find that

\[
\hat{S}_x^2 = \sum_i (\hat{S}_x^i)^2 + \sum_{i \neq j} \hat{S}_x^i \hat{S}_x^j
\]

so that on taking the trace with \( \hat{\rho}_R \) and using Eqs. (353) we get after applying the commutation rules \([\hat{e}, \hat{e}^\dagger] = 1 \) (\( \hat{e} = \hat{a} \) or \( \hat{b} \))

\[
\langle \hat{S}_x^2 \rangle_R = \sum_i \langle (\hat{S}_x^i)^2 \rangle_R + \sum_{i \neq j} \langle \hat{S}_x^i \rangle_R \langle \hat{S}_x^j \rangle_R
\]

As we also have

\[
\langle \hat{S}_z \rangle_R = \sum_i \langle \hat{S}_x^i \rangle_R \quad \langle \hat{S}_x \rangle_R = \sum_i \langle \hat{S}_x^i \rangle_R
\]

using Eqs. (353) and we see finally that the variance \( \langle \Delta \hat{S}_x^2 \rangle_R \) is

\[
\langle \Delta \hat{S}_x^2 \rangle_R = \sum_i \langle (\hat{S}_x^i)^2 \rangle_R - \sum_i \langle \hat{S}_x^i \rangle_R^2
\]

all the terms with \( i \neq j \) cancelling out. and therefore from Eq. (352)

\[
\langle \Delta \hat{S}_x^2 \rangle_R \geq \sum R P_i \sum_i \left( \langle (\hat{S}_x^i)^2 \rangle_R - \langle \hat{S}_x^i \rangle_R^2 \right)
\]

But using (354)

\[
(\hat{S}_x^i)^2 = \frac{1}{4} (\hat{b}_i^\dagger \hat{b}_i \hat{a}_i \hat{a}_i^\dagger + \hat{b}_i^\dagger \hat{a}_i \hat{a}_i \hat{b}_i^\dagger + \hat{a}_i^\dagger \hat{b}_i \hat{b}_i \hat{a}_i^\dagger + \hat{a}_i^\dagger \hat{a}_i \hat{b}_i \hat{b}_i^\dagger)
\]

\[
\langle (\hat{S}_x^i)^2 \rangle_R = \frac{1}{4} (\langle \hat{b}_i \hat{b}_i \rangle_R + \langle \hat{a}_i \hat{a}_i \rangle_R) + \frac{1}{2} (\langle (\hat{a}_i^\dagger \hat{a}_i) \rangle_R \langle \hat{b}_i \hat{b}_i \rangle_R)
\]

and

\[
\langle \hat{S}_x^i \rangle_R = 0
\]

so that

\[
\langle \Delta \hat{S}_x^2 \rangle_R \geq \sum R P_i \sum_i \left( \frac{1}{4} (\langle \hat{b}_i \hat{b}_i \rangle_R + \langle \hat{a}_i \hat{a}_i \rangle_R) + \frac{1}{2} (\langle (\hat{a}_i^\dagger \hat{a}_i) \rangle_R \langle \hat{b}_i \hat{b}_i \rangle_R) \right)
\]

Now using (354)

\[
\langle \hat{S}_x^i \rangle_R = \frac{1}{2} (\langle \hat{b}_i \hat{b}_i \rangle_R - \langle \hat{a}_i \hat{a}_i \rangle_R)
\]

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\[ \langle \hat{S}_z \rangle = \sum_R P_R \sum_i \langle \hat{S}_z^i \rangle_R \]

\[ \frac{1}{2} |\langle \hat{S}_z \rangle| = \frac{1}{2} \sum_R P_R |\sum_i \frac{1}{2} (\langle \hat{b}^i \hat{b}^i \rangle_R - \langle \hat{a}^i \hat{a}^i \rangle_R)\rangle| \]

\[ \leq \sum_R P_R \frac{1}{4} \sum_i |(\langle \hat{b}^i \hat{b}^i \rangle_R - \langle \hat{a}^i \hat{a}^i \rangle_R)| \]

\[ \leq \sum_R P_R \frac{1}{4} \sum_i (\langle \hat{b}^i \hat{b}^i \rangle_R + \langle \hat{a}^i \hat{a}^i \rangle_R) \]

(365)

and thus

\[ \langle \Delta \hat{S}_z^2 \rangle - \frac{1}{2} |\langle \hat{S}_z \rangle| \]

\[ \geq \sum_R P_R \sum_i \left( \frac{1}{4} (\langle \hat{b}^i \hat{b}^i \rangle_R + \langle \hat{a}^i \hat{a}^i \rangle_R) + \frac{1}{2} (\langle \hat{b}^i \hat{b}^i \rangle_R \langle \hat{b}^i \hat{b}^i \rangle_R) \right) \]

\[ - \sum_R P_R \frac{1}{4} \sum_i (\langle \hat{b}^i \hat{b}^i \rangle_R + \langle \hat{a}^i \hat{a}^i \rangle_R) \]

\[ = \sum_R P_R \frac{1}{2} \sum_i (\langle \hat{a}^i \hat{a}^i \rangle_R \langle \hat{b}^i \hat{b}^i \rangle_R) \]

\[ \geq 0 \]

(366)

A similar proof shows that \( \langle \Delta \hat{S}_x^2 \rangle - \frac{1}{2} |\langle \hat{S}_x \rangle| \geq 0 \) for the non-entangled state of all 2N modes.

This shows that for the general non-entangled state with all modes \( \hat{a}_i \) and \( \hat{b}_i \) as the sub-systems, the variances for two of the spin fluctuations \( \langle \Delta \hat{S}_z^2 \rangle \) and \( \langle \Delta \hat{S}_y^2 \rangle \) are both greater than \( \frac{1}{2} |\langle \hat{S}_z \rangle| \), and hence there is no spin squeezing for \( \hat{S}_x \) or \( \hat{S}_y \). Note that as \( |\langle \hat{S}_y \rangle| = 0 \), the quantity \( \sqrt{(1 |\langle \hat{S}_{\perp 1} \rangle|^2 + |\langle \hat{S}_{\perp 2} \rangle|^2)} \)

is the same as \( |\langle \hat{S}_x \rangle| \), so the alternative criterion in Eq. (360) is the same as that in Eq. (116), which is used here.

For the other spin fluctuation \( \langle \Delta \hat{S}_x^2 \rangle \) since we have

\[ \langle \hat{S}_x \rangle = \sum_R P_R \langle \hat{S}_x \rangle_R = 0 \]

\[ \langle \hat{S}_y \rangle = \sum_R P_R \langle \hat{S}_y \rangle_R = 0 \]

(367)

then the other two uncertainty relationships just give \( \langle \Delta \hat{S}_y^2 \rangle \langle \Delta \hat{S}_x^2 \rangle \geq 0 \);

\( \langle \Delta \hat{S}_z^2 \rangle \langle \Delta \hat{S}_x^2 \rangle \geq 0 \), so spin squeezing in \( \hat{S}_z \) is meaningless.

Hence we have shown that for a non-entangled physical state for all the 2N modes \( \hat{a}_i \) and \( \hat{b}_i \),

\[ \langle \Delta \hat{S}_x^2 \rangle \geq \frac{1}{2} |\langle \hat{S}_x \rangle| \quad \text{and} \quad \langle \Delta \hat{S}_y^2 \rangle \geq \frac{1}{2} |\langle \hat{S}_y \rangle| \]

(368)

137
so that spin squeezing in either $\hat{S}_x$ or $\hat{S}_y$ requires entanglement.

### 16.2 Variance $\left< \Delta \hat{S}_z^2 \right>$

Here we will see if the modified approach to Sorensen et al can lead to a useful inequality for $\left< \Delta \hat{S}_z^2 \right>$ that applies when non-entangled states are those when the *pairs* of modes $\hat{a}_i$ and $\hat{b}_i$ are the separate sub-systems. We will attempt to follow the approach used by Sorensen et al when identical particles $i$ were regarded as the sub-systems.

Now the general non-entangled state will be

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^1 \otimes \hat{\rho}_R^2 \otimes \hat{\rho}_R^3 \otimes \ldots$$

(369)

where the $\hat{\rho}_R^i$ are now of the form given in Eq. (213) and the conditions in Eq. (354) no longer apply. The Fock states are of the form $|N_{ia}\rangle \otimes |N_{ib}\rangle$ for the pair of modes $\hat{a}_i$ and $\hat{b}_i$, and for this Fock state the total occupancy of the pair of modes is $N_i = N_{ia} + N_{ib}$. From the super-selection rule the density operator $\hat{\rho}_R^i$ for the $i$th pair of modes $\hat{a}_i$ and $\hat{b}_i$ is diagonal in the total occupancy. For $N_i = 0$ there is one non zero matrix element $\langle (0)_{ia} \otimes (0)_{ib} | \hat{\rho}_R^i | (0)_{ia} \otimes (0)_{ib} \rangle$. For $N_i = 1$ there are four non zero matrix elements, which may be written

$$\begin{align*}
\langle (1)_{ia} \otimes (0)_{ib} | \hat{\rho}_R^i | (1)_{ia} \otimes (0)_{ib} \rangle &= \rho_{ia}^i \\
\langle (1)_{ia} \otimes (0)_{ib} | \hat{\rho}_R^i | (0)_{ia} \otimes (1)_{ib} \rangle &= \rho_{ib}^i \\
\langle (0)_{ia} \otimes (1)_{ib} | \hat{\rho}_R^i | (1)_{ia} \otimes (0)_{ib} \rangle &= \rho_{ba}^i \\
\langle (0)_{ia} \otimes (1)_{ib} | \hat{\rho}_R^i | (0)_{ia} \otimes (1)_{ib} \rangle &= \rho_{bb}^i
\end{align*}$$

(370)

For $N_i = 2$ there are nine non zero matrix element $\langle (2)_{ia} \otimes (0)_{ib} | \hat{\rho}_R^i | (2)_{ia} \otimes (0)_{ib} \rangle$, ..., $\langle (0)_{ia} \otimes (2)_{ib} | \hat{\rho}_R^i | (0)_{ia} \otimes (2)_{ib} \rangle$ and the number increases with $N_i$.

If we restrict ourselves to general entangled states where $N_i = 1$ for all pairs of modes, then the density operator $\hat{\rho}_R^i$ is of then form

$$\hat{\rho}_R = \rho_{aa}^i \langle 1 |_{ia} \otimes | 0 \rangle_{ib} \langle 0 |_{ib} \rangle + \rho_{bb}^i \langle 0 |_{ib} \otimes | 1 \rangle_{ib} \langle 1 |_{ib} \rangle$$

(371)

In addition Hermitian, positivity, unit trace $Tr(\hat{\rho}_R^i) = 1$ and $Tr(\hat{\rho}_R^i)^2 \leq 1$ can be used as in Eq (357) to parameterise the matrix elements in (370).

$$\begin{align*}
\rho_{aa}^i &= \sin^2 \alpha_i \\
\rho_{bb}^i &= \cos^2 \alpha_i \\
\rho_{ab}^i &= \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i} \exp(i \phi_i) \\
\rho_{ba}^i &= \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i} \exp(-i \phi_i)
\end{align*}$$

(372)
The expectation values for the spin operators \( \hat{S}^x_i, \hat{S}^y_i \) and \( \hat{S}^z_i \) associated with the \( i \)th pair of modes are then

\[
\begin{align*}
\langle \hat{S}^x_i \rangle_R &= \text{Tr}(\hat{\rho}^i_R \frac{1}{2} (\hat{b}^\dagger_i \hat{a}_i + \hat{a}^\dagger_i \hat{b}_i)) \\
&= \frac{1}{2} (\rho^i_{ab} + \rho^i_{ba}) \\
\langle \hat{S}^y_i \rangle_R &= \frac{1}{2i} (\rho^i_{ab} - \rho^i_{ba}) \\
\langle \hat{S}^z_i \rangle_R &= \frac{1}{2} (\rho^i_{bb} - \rho^i_{aa})
\end{align*}
\]

which are of exactly the same form as in Eq. (346) as in the Appendix derivation of the original Sorensen et al. [45] results based on treating identical particles as the sub-systems. The proof however is now different and rests on restricting the states \( \hat{\rho}^i_R \) to each containing exactly one boson.

The remainder of the proof is exactly the same as in Appendix and we find that

\[
\langle \Delta \hat{S}^2_z \rangle \geq \frac{1}{N} \left( \langle \hat{S}^2_x \rangle + \langle \hat{S}^2_y \rangle \right)
\]

for non-entangled pairs of modes \( \hat{a}_i \) and \( \hat{b}_i \). Thus when the interpretation is changed so that the separate sub-systems are these pairs of modes, it follows that spin squeezing requires entanglement of all the mode pairs.
17 Appendix 9 - Heisenberg Uncertainty Principle Results

Here we derive the results in SubSection 5.4 leading to inequalities for the variance $\langle \Delta \hat{J}_x^2 \rangle$ considered as a function of $|\langle \hat{J}_z \rangle|$ for states where the spin operators are chosen such that $\langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0$.

From the Schwarz inequality $\langle \hat{J}_z \rangle^2 \leq \langle \hat{J}_z^2 \rangle$ so that

$$\langle \hat{J}_x^2 \rangle + \langle \hat{J}_y^2 \rangle \leq \langle \hat{J}_x^2 \rangle + \langle \hat{J}_y^2 \rangle + \langle \hat{J}_z^2 \rangle = J(J+1) \quad (375)$$

giving Eq. (225). Subtracting $\langle \hat{J}_x^2 \rangle = \langle \hat{J}_y^2 \rangle = 0$ from each side gives

$$\langle \Delta \hat{J}_x^2 \rangle + \langle \Delta \hat{J}_y^2 \rangle + \langle \hat{J}_z^2 \rangle \leq J(J+1) \quad (376)$$

Substituting for $\langle \Delta \hat{J}_y^2 \rangle$ from the Heisenberg uncertainty principle result in Eq. (226) gives

$$\langle \Delta \hat{J}_x^2 \rangle - \left( J(J+1) - \langle \hat{J}_z \rangle^2 \right) \langle \Delta \hat{J}_z^2 \rangle + \frac{1}{4} \xi \langle \hat{J}_z \rangle^2 \leq 0 \quad (377)$$

The left side is a parabolic function of $\langle \Delta \hat{J}_z \rangle$ and for this to be negative requires $\langle \Delta \hat{J}_z \rangle$ to lie between the two roots of this function, giving

$$\langle \Delta \hat{J}_x^2 \rangle \geq \frac{1}{2} \left\{ (J(J+1) - \langle \hat{J}_z \rangle^2) - \sqrt{(J(J+1) - \langle \hat{J}_z \rangle^2)^2 - \xi \langle \hat{J}_z \rangle^2} \right\} \quad (378)$$

$$\langle \Delta \hat{J}_x^2 \rangle \leq \frac{1}{2} \left\{ (J(J+1) - \langle \hat{J}_z \rangle^2) + \sqrt{(J(J+1) - \langle \hat{J}_z \rangle^2)^2 - \xi \langle \hat{J}_z \rangle^2} \right\} \quad (379)$$

which are the required inequalities in Eq. (227) and (228).
18 Figure Captions

Figure 1. Bloch vector and spin fluctuations shown for original spin operators.

Figure 2. Regions in the $< \Delta \hat{J}_z^2 >$ versus $| < \hat{J}_z > |$ plane (shown shaded) for states that satisfy (a) the spin squeezing inequality Eq. (229) (b) the smaller Heisenberg uncertainty principle inequality Eq. (227) and (c) the larger HUP inequality Eq. (228). The case shown is for $J = 1000$ and HUP factor $\xi = 1$. Both $< \Delta \hat{J}_z^2 >$ and $| < \hat{J}_z > |$ are in units of $J$. The spin operators are chosen so that $< \hat{J}_x >= < \hat{J}_y >= 0$.

Figure 3. As in Figure 2, but with $J = 1000$ and HUP factor $\xi = 10.0$.

Figure 3. As in Figure 2, but with $J = 1$ and HUP factor $\xi = 10.0$. 
Figure 1:
Figure 2:
This figure "SpinSqgFig1.jpg" is available in "jpg" format from:

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