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Invited Comment

Quantum entanglement for systems of identical bosons: I. General features

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Abstract

These two accompanying papers are concerned with two mode entanglement for systems of identical massive bosons and the relationship to spin squeezing and other quantum correlation effects. Entanglement is a key quantum feature of composite systems in which the probabilities for joint measurements on the composite sub-systems are no longer determined from measurement probabilities on the separate sub-systems. There are many aspects of entanglement that can be studied. This two-part review focuses on the meaning of entanglement, the quantum paradoxes associated with entangled states, and the important tests that allow an experimentalist to determine whether a quantum state—in particular, one for massive bosons is entangled. An overall outcome of the review is to distinguish criteria (and hence experiments) for entanglement that fully utilize the symmetrization principle and the super-selection rules that can be applied to bosonic massive particles. In the first paper (I), the background is given for the meaning of entanglement in the context of systems of identical particles. For such systems, the requirement is that the relevant quantum density operators must satisfy the symmetrization principle and that global and local super-selection rules prohibit states in which there are coherences between differing particle numbers. The justification for these requirements is fully discussed. In the second quantization approach that is 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 work mainly focuses on the two mode entanglement for massive bosons, but is put in the context of tests of local hidden variable theories, where one may not be able to make the above restrictions. The review provides the detailed arguments necessary for the conclusions of a recent paper, where the question of how to rigorously demonstrate the entanglement of a two-mode Bose–Einstein condensate (BEC) has been examined. In the accompanying review paper (II), we consider spin squeezing and other tests for entanglement that have been proposed for two-mode bosonic systems. We apply the approach of review (I) to determine which tests, and which modifications of the tests, are useful for detecting entanglement in massive bosonic (BEC), as opposed to photonic, systems. Several

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new inequalities are derived, a theory for the required two-mode interferometry is presented, and key experiments to date are analyzed.

S Online supplementary data available from stacks.iop.org/ps/92/023004/mmedia

Keywords: entanglement, identical massive bosons, super-selection rules, spin squeezing, correlation, quadrature squeezing, phase reference

1. Introduction

Since the paradoxes of Einstein–Podolski–Rosen (EPR) [1], Schrödinger [2, 3] and Bell [4], *entanglement* has been recognized as a key feature that distinguishes quantum physics from classical physics. Entangled quantum states underlie the EPR and Bell paradoxes, which reveal the conflict between quantum mechanics and local realism, and the famous Schrödinger cat paradox, where a cat is apparently prepared in a state simultaneously both dead and alive. Entanglement not only provides a way to rigorously test quantum principles, but is the basis for the many quantum information tasks like quantum cryptography. Despite the fundamental interest, there have been only a few experimental tests of entanglement for systems of massive particles. Yet, the substantial recent progress in cooling atomic systems, in particular to form Bose–Einstein condensates (BECs), makes such entanglement tests much more feasible.

In this review (I), we explain the meaning of entanglement, and examine how to verify entanglement, for systems of identical boson particles. This leads us to focus on symmetrization and superselection rules, and to consider their implication for entanglement criteria when applied to massive bosonic particles. This paper provides the theoretical background for a recent paper [5] and a subsequent paper (II) [6] that analyses the suitability of specific criteria, new and old, to detect entanglement in *massive* bosonic systems, and applies the criteria to interpret experimental findings.

As well as reviewing the topic and presenting some new results in paper II, these two articles are intended as comprehensive papers for post docs and postgraduates who are changing field or starting work in a new one and need to gain a thorough understanding of the present state of knowledge. With this aim in mind we have not followed the conventional approach in review articles of merely quoting formulae and giving references, but instead have presented full proofs of the key results. To really understand a field, we believe it is necessary to work through the derivations. However, in order to shorten the main body of the articles, we have included many of the details in appendices. The appendices are available as online supplementary material (stacks.iop.org/ps/92/023004/mmedia). References [108]–[122] are discussed therein.

1.1. Entanglement: definitions and historical context

Entanglement 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 measured values 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 then 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. The set of non-entangled states must allow *all* possible quantum states for the given sub-system, but 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 quantum 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 [7]. The notion of *quantum 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 3. Entangled states underlie a number of effects that cannot be interpreted in terms of classical physics, including *spin squeezing* and non-local measurement *correlations*-such as for the EPR *paradox* and violations of *Bell Inequalities* [1, 2, 4, 8–11]. The quantum theory of measurement [12–15] invokes entangled states of the system and measuring apparatus as key concepts in the theory. More recently, entangled states have been recognized 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 [15–20].

It would be pointless to characterize 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 section 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. In general, entangled states do not exhibit this feature of separable probabilities, and it is this key non-separability feature that led Schrödinger to call these states 'entangled'. Where the sub-systems are spatially separated, one can define spacelike separated local measurement events on each. This was historically the reason why the sub-systems and their measurements are often referred to as *local*. The EPR paper [1] suggested the possibility that although the predictions of quantum theory were correct, the theory was *incomplete* and there was an underlying reality in the form of *classical hidden variables*. Averaging over the unknown values of the hidden variables would be required to produce the same measurement probabilities as quantum theory. *Local hidden variable* (LHV) theories are discussed in section 2.5, and it will be seen that the joint probabilities for measurements of sub-system physical quantities are of the same form as for *separable* states. As will be seen in sections 2.6 and 2.7, states for which local measurements can be described by LHV theories satisfy Bell inequalities. This includes the separable states. States described by a LHV theory are referred to as *Bell-local* states—all other states are *Bell non-local* states. If a state violates a Bell inequality it must be entangled, since separable states are Bell local. Hence there is a direct link between Bell inequality violations and both the *failure* of LHV theories and the presence of *entanglement*. The fact that *certain* entangled states do not exhibit the feature of separable probabilities shown in classical LHV theories highlights entanglement being a *non-classical* feature found in composite systems.

Note that although an EPR or Bell inequality violation requires the quantum state to be entangled, there are examples of mixed entangled states that do *not* violate a Bell inequality. For *pure* states of qubits Gisin [21] showed that entangled states always violated Bell inequality, but for *mixed* states Werner [7] and others [22–24] have shown there are entangled states (*Werner states* [17]) for which a hidden variable theory (HVT) can be constructed that gives the same joint probability function for measurement outcomes as quantum theory. These specific entangled states will therefore satisfy Bell inequalities, so *some* entangled states are Bell local. For completeness, the important mixed entangled states considered by Werner are described in appendix A. At present detailed LHV theories have not been developed which can independently determine the LHV measurement probability functions for the sub-systems as a function of the hidden variables, but as Werner showed for certain composite states that such measurement probability functions could be found which would be consistent with the overall quantum probability functions for joint measurements on the composite system state. So in that sense the LHV theory could account for the results from quantum theory even though at present it does not have the predictive power of quantum theory—even for states not violating Bell inequalities.

The issue of how best to treat the quantum aspects of *correlations* in measurement outcomes in composite quantum systems is still an active area of research and is beyond the scope of these two papers. Quantum entanglement is clearly relevant to the discussion, but concepts such as *quantum discord* [25, 26] and EPR steering [1, 3, 27–29] are now being used to describe quantum correlations. The link between these concepts is discussed in [30]. In these recent discussions of quantum correlation, it turns out that some separable states are regarded as exhibiting quantum correlations. In [27–29] the concept of *local hidden state* (LHS) is introduced within LHV theory to describe states of sub-systems for which a density operator exists that is determined by the hidden variables, and which can be used to account for measurements on the sub-system in accordance with standard quantum expressions. It can also be used [27] to construct a quantum state for the sub-system with the LHS that is the conditional quantum state obtained resulting from the outcome of a local measurement on the other sub-system. The absence of such a LHS results in EPR steering being possible—a paradoxical non-classical effect identified by both Einstein *et al* [1] and by Schrödinger [3]. In [27–29] it is seen that some entangled Bell local states exhibit EPR steering, in addition to the Bell non-local states. In [27] the parameter regions for *Werner states* being (a) separable (b) entangled, Bell local but non-steerable (c) entangled, Bell local and steerable (d) entangled, Bell non-local and steerable are determined, along with similar considerations for so-called *isotropic states*. The development of tests for EPR steering is still an active area of research [31, 32].

It is now generally recognized that entanglement is a *relative* concept [17, 33–37] 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. A simple example often cited is that for the hydrogen atom [35], a system made up of two distinguishable particles, a proton and an electron. Here the energy eigenstates are non-entangled if the sub-systems refer to the center of mass of the entire atom and the relative position of the electron and the proton, but which would be entangled if the sub-systems were the positions of the electron and proton. It could be argued that the center of mass and the relative position are not really independent sub-systems—one always accompanies the other—but as unrelated center of mass and relative position quantum states can be prepared, they can be regarded as distinct sub-systems. The individual positions of the electron and the proton are also distinct sub-systems, and the ground state of the hydrogen atom is indeed entangled—the electron position is tightly correlated with the proton position. Another example involves two different choices of single particle states in a two mode BEC—a system with a

large number of identical particles. The issue of defining sub-systems will be dealt with below, but taking the original two sub-systems to be bosonic modes (or single particle states) denoted $|\phi_A\rangle$ and $|\phi_B\rangle$, a well known N boson entangled state of these two modes A and B (with mode annihilation operators $\hat{a}$ and $\hat{b}$) is the *binomial state* given by $|\Phi\rangle = ((\cos\theta\,\exp(\mathrm{i}\chi/2)\hat{a} + \sin\theta\,\exp(-\mathrm{i}\chi/2)\hat{b}^{\dagger})^N/\sqrt{N!}\;|0\rangle$ (see [38] and paper II, section 3.6) which is a quantum superposition of Fock states $(\hat{a}^{\dagger})^k/\sqrt{k!}\;(\hat{b}^{\dagger})^{N-k}/\sqrt{(N-k)!}\;|0\rangle$ with $k = 0,\ldots,N$. Introducing new modes via $\hat{c} = (\cos\theta\,\exp(\mathrm{i}\chi/2)\hat{a} + \sin\theta\,\exp(-\mathrm{i}\chi/2)\hat{b})$ and $\hat{d} = (-\sin\theta\,\exp(\mathrm{i}\chi/2)\hat{a} + \cos\theta\,\exp(-\mathrm{i}\chi/2)\hat{b})$ we see that we can also write $|\Phi\rangle = (\hat{c}^{\dagger})^N/\sqrt{N!}\;|0\rangle$, so that the same quantum state is a separable state if the sub-systems are chosen to be the new modes C and D. Another example is the ground state of the single mode non-interacting BEC trapped in a harmonic oscillator (HO) potential. This is a separable state, with all bosons in the lowest energy mode if the sub-systems are chosen as the HO modes. However, if single particle position states spatially localized in two different regions are chosen as two sub-systems, then the same ground state for the identical particle system is spatially entangled, as pointed out by Goold *et al* [39].

1.2. Measures and tests for entanglement

Various *measures* of entanglement have been defined for certain types of quantum state—see [17, 18, 26, 36, 37, 40, 41], 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 [17, 18], this measure is of importance to *quantum information science*. Measurements of entanglement based on *Renyi entropy* and *purity* are discussed in [42–44]. Another entanglement measure is *particle entanglement*, defined by Wiseman *et al* [40, 45, 46] for identical particle systems and based on projecting the quantum state onto states with definite particle numbers. One of the problems with entanglement measures is that there is often no simple way to measure the quantities required.

In the case of *bipartite* entanglement in qubit systems [47, 48] obtained a sufficient condition for a quantum state to be entangled (*PPT condition*) (see [36, 37], for details). Suppose the density operator $\hat{\rho}$ is changed into $\hat{\rho}^T$ by mapping the matrix elements associated with one of the sub-systems into their *transpose*. Then provided the new operator $\hat{\rho}^T$ is a valid density operator (with real, non-negative eigenvalues that add to unity), the original density operator represents a separable state. Thus, if it is shown that some of the eigenvalues of $\hat{\rho}^T$ are negative, then the state $\hat{\rho}$ is entangled. However, it is often not practical to use this as an entanglement test for systems with large numbers of basis states, as it requires being able to measure all the density matrix elements. It was also later realized [49] that in general, the PPT condition was not a necessary condition for entanglement, apart from cases of 2×2 and 2×3 subsystems—that is, showing that $\hat{\rho}^T$ has only positive eigenvalues will not guarantee that $\hat{\rho}$ is separable, as counter-examples for 2×4 and 3×3 subsystems showed. Toth and Guhne [50] considered the effect of permutational symmetry on the PPT condition for entanglement in bipartite systems.

Although not directly related 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 [36, 37, 40]. These are in the form of *inequalities* for *variances* and *mean values* for certain physical quantities, which are dependent on the inequalities applying 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. In the case of entanglement witnesses, the idea is to find a Hermitian operator $\widehat{W}$ such that for separable states $Tr(\widehat{W}\hat{\rho}) \geqslant 0$, so that if $Tr(\widehat{W}\hat{\rho}) < 0$ the state must be entangled. Here we note that the density operator occurs linearly when evaluating the quantities involved. Some of the *correlation* tests discussed in paper II are cases involving entanglement witnesses. However, in more general tests for entanglement the density operator appears nonlinearly. For example, a *spin squeezing* test for entanglement may require showing that the variance for a spin operator is less than a multiple of the magnitude of the mean value of another spin operator—thus for example $\langle\Delta\hat{S}_x^2\rangle < |\langle\hat{S}_z\rangle|/2$. This could be written as $\mathrm{Tr}((\hat{S}_x^2 \pm \hat{S}_z/2)\hat{\rho}) - (\mathrm{Tr}(\hat{S}_x)\hat{\rho}))^2 < 0$, which is of a more general form than for an entanglement witness. Nonlinear tests are discussed in [37]. One of the advantages of entanglement tests is that the quantities involved can be measured. It cannot be emphasized enough that these tests provide *sufficiency conditions* for establishing that a state is entangled. So if the test is satisfied we can conclude that the state is not separable. The failure of a test does *not* mean that the state is not entangled—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 section 3.5 of the accompanying paper II shows. A significant number of such inequalities have now been proposed and such signatures of entanglement are the primary focus of the accompanying 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 emphasize 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.

1.3. Particle versus mode entanglement

These two papers deal with *identical* particles—bosons or fermions. In the *second quantization* 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*. We now take into account the situation where systems of *identical particles* are involved. This requires us to give special consideration to the requirement that quantum states in such cases must conform to the *symmetrization principle*. What sub-systems are possible must take into account that entanglement requires the specification of sub-systems that are *distinguishable* from each other and on which *measurements* can be made. In addition, the sub-systems must be able to exist as *separate* systems which can be prepared in quantum states for that sub-system alone. These key requirements that the sub-systems must be distinguishable, susceptible to measurements and can exist in separate quantum states are necessary for the concept of entanglement to make *physical* sense, and have important consequences for the choice of sub-systems when identical particles are involved. These three key logical requirements for sub-systems rule out considering *labeled identical particles* as sub-systems and lead to the conclusion that sub-systems must be *modes*. Thus 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 [17, 33–35, 51, 52]. In this approach, *particles* are associated with 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 quantization* 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 2 of accompanying paper II. Modes can often be categorized as *localized* modes, where the corresponding single particle wavefunction is confined to a restricted spatial region, or may be categorized as *delocalized* modes, where the opposite applies. Single particle HO states are an example of localized modes, momentum states are an example of delocalized modes. This distinction is significant when phenomena such as EPR violations and teleportation are considered.

However, even if the system consists entirely of *distinguishable* particles we can still regard the sub-systems as collections of modes. Each distinguishable particle is still associated with a set of single particle states or modes (momentum eigenstates, HO eigenstates, etc) that can be occupied. More general states associated with a single particle may be quantum superposition states of those with a single particle occupancy of the modes. If the overall system consists of a number of distinguishable particles each of which is considered as a sub-system, then each such sub-system can equally be regarded as the set of modes associated with the particular distinguishable particle. Overall system states involving just one particle of each type would be simultaneous eigenstates of the number operators for each of the distinguishable particles, with an eigenvalue of unity corresponding to there being only one particle of each type. The second quantization approach can still be used, but is somewhat superfluous when the modes for each particle are only occupied once.

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 [53] 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.

1.4. Symmetrization and super-selection rules (SSRs)

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 [7] in which the separable states are those that can be prepared by *local operations* and *classical communication* (LOCC). This approach is adopted by other authors, see for example [28, 54, 55]. However, in other papers—see for example [56, 57] so-called separable non-local states are introduced, where the authors do not incorporate the requirement of LOCC in their definition of separable states. (See section 3.4.2 for an example.)

In the present LOCC based paper it is contended that the *density operators* both for the *quantum states* of the overall

system and those for the non-entangled (local) sub-systems in the context of *non-entangled states* must be compatible with certain principles and rules that have been found to be both necessary and sufficient for understanding *physical experiments* in non-relativistic many-body systems. In some other work (discussed below) this has not been the case. A key feature required of all quantum states for systems involving *identical particles*, entangled or not is that they satisfy the *symmetrization principle* [58]. 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). If the system consists entirely of *distinguishable particles* then the symmetrization principle is not relevant. In addition, super-selection rules (SSR) [59] only allow density operators which have *zero coherences* between states with *differing total numbers* of particles to represent valid *quantum states*, and this will be taken into account for *all* quantum states of the overall system, entangled or not. This is referred to as the *global particle number* SSR 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 quantum states, a so-called *local particle number* SSR will *also* be applied to the density operators describing each of the *sub-systems*. These sub-system density operators 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 SSR. 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* [54, 60] as one of several approaches for defining entangled states. However, other authors such as [56, 57] state on the contrary that states where the sub-system density operators do *not* conform to the local particle number SSR *are* still separable, others such as [61, 62] do so by implication—the latter papers applied to atomic as well as photon modes. So in these two papers 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 SSRs on particle numbers be applied to the *overall* quantum 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. As Werner's [7] original LOCC based approach invoked the idea that separate sub-system states could be created, we contend that applying the constraints of symmetrization and local particle number SSRs for the sub-system states that occur in separable states is consistent with Werner's approach, even though he did not consider the specific physics of identical massive particle systems at the time.

Note that for systems entirely consisting of N *distinguishable* particles the SSRs are still true, but are now *superfluous*. Each sub-system is the set of modes or *one particle states* of the *specific* distinguishable particle and the overall state is an N particle state in which the sub-systems only contain *one* particle. Consequently there are no sub-system or system coherences between states with differing particle number.

The detailed reasons for adopting the viewpoint that the entanglement criteria be compliant with the requirement of the local particle number SSR for the sub-system are set out below. As will be seen, the local particle number SSR 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 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 sub-system quantum states. As mentioned before, the general definition of non-entangled states based on LOCC preparation processes was first suggested by Werner [7]. Apart from the papers by Bartlett *et al* [54, 60] 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 [56, 57]. However, the idea of considering whether sub-system states should satisfy the local particle number SSR has been presented in several papers—[54, 56, 57, 60, 63–65], 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 [56], multicopy distillation [54], mechanical work and accessible entanglement [63, 64] and Bell inequality violation [65]. The consequences for entanglement of applying this SSR requirement to the sub-system density operators are quite *significant*, and in the accompanying paper II 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 (accompanying paper II) 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 symmetrization principle and the SSRs.

It is worth emphasizing that requiring the sub-system density operators satisfy the local particle number SSR means that there are less states than otherwise 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 appendix C of paper II, where the sub-systems are restricted to one boson states.

The *symmetrization* requirement for systems involving identical particles is well established since the work of Dirac

There are two types of justification for applying the SSR*s* for systems of identical particles (both massive and otherwise). The *first* approach for invoking the superselection rule to exclude quantum superposition states with differing numbers of identical particles is based on simple considerations and may be summarized as:

(1) No way is known for creating such SSR non-compliant states.

(2) No way is known for measuring the properties of such states.

(3) Coherence and interference effects can be understood in terms of SSR compliant states.

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 [40, 56, 57, 60, 63, 64, 66–71]. This approach will be described in section 3.2 and appendix K, the key idea being that SSR are a consequence of considering the description of a quantum state by a real observer (Charlie) whose phase reference frame has an *unknown phase difference* from that of a hypothetical observer (Alice), both studying the same system. Alice is assumed to possess a phase reference frame such that her description of the quantum state of the system violates the SSR. Charlie, on the other hand is an actual observer with no such phase reference frame. Thus, while Alice's description of the system involves a quantum state may violate the SSR, the description of the same system by Charlie will involve a quantum state that is SSR compliant. In the main part of this paper the density operator $\widehat{\rho}$ used to describe the various quantum states will be that of the external observer (Charlie). Note that if well-defined phase references do *exist* and the relationship between them is *known*, then the SSR can be challenged (see sections 3.3 and appendix K), but this situation does not apply in the case of massive bosons (or fermions).

It should be noted that both of these justifications for applying the SSR are dependent on what is practical in terms of measurements in *non-relativistic* quantum physics. Here the situation is much clearer for systems of massive particles such as atoms than for massless particles such as photons. Applying SSR for photons is discussed in section 3.2.3 and in appendix L.

However, to allow for quantum 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 is an unnecessary feature to add to the non-relativistic quantum physics of many body systems or to quantum optics. 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. The quantum state is intended to specify what is known about a quantum system and how it was prepared. It is used to determine the probabilities for possible measurements on the system. Clearly there is no point in including non-SSR compliant terms in the density operator for the quantum state. Such terms would neither allow for possible preparation processes, or contribute to measurement probabilities associated with physical effects. 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 SSR 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 SSR for the overall system it would be *inconsistent* not to apply it to the sub-system as well. As we will see, for separable states the requirement that the overall state is SSR compliant generally implies that the sub-system states are SSR compliant—though in some special cases this is not the case (see section 4.3.3 of paper II). The *onus* is on those who wish to ignore the SSR for the separate sub-systems 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 SSRs has however been challenged (see section 3.2) on the basis that SSRs 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 3 and in appendix M an analysis of these objections to the SSR is presented, and in appendix K 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 sceptic who wishes to ignore the SSRs in the definition of entanglement—and consequently only consider as valid tests for entanglement where SSR compliance is *not* used in their derivation—needs to carry out a research program analogous to that which resulted in *parity non-conservation* becoming a basic feature of *weak interaction theory*. The successful incorporation of parity non-conservation involved first proposing (on symmetry grounds) possible interactions in which parity was not conserved, second working out possible experiments that could confirm parity non-conservation and third carrying out key experiments that did confirm this. At this stage no such work in regard to SSR violation in the non-relativistic many body physics of massive particles has been carried out or is likely to be in the near future. As we will see in paper II, none of the experimental methods for entanglement tests that we examine can detect SSR non-compliance—none involve a suitable *phase reference*. To ignore SSR in non-relativistic entanglement theory and experiment on the grounds of scepticism would be analogous to including parity non-conservation in quantum chemistry or atomic physics—areas which are well-understood in terms of parity being conserved (apart from the well-known parity violating effects of external electric fields). When and if SSR violation in non-relativistic many body physics is found would then be the time to revise the definition of quantum entanglement. In these two papers we will utilize the definition of entanglement and derive tests based on SSR compliance, though of course recognizing that there are also tests that do not require SSR compliance which are *also* valid for SSR compliant states. Although other definitions of entanglement will be considered for comparison, to

avoid confusion the SSR compliant definition will be the one which we mean when we refer to entanglement.

A further sound scientific argument can be presented in favor of studying SSR compliant entanglement tests (as is our aim in these papers (I) and (II)). This involves a consideration of what can be concluded from such tests by supporters or sceptics of SSR. For example, one such test (see paper II) involves spin squeezing in two mode systems. If the state is separable *and* the sub-system states comply with local SSR then there is *no* spin squeezing. However, if experimental tests *do* demonstrate spin squeezing, then what can we conclude? The supporters of SSR compliance being required for the sub-systems would conclude that the state was not separable and hence *entanglement* is present between the subsystems. On the other hand, the sceptic who does not believe local SSR compliance is required would have no option but to conclude *either* that entanglement is present between the subsystems *or* (if they argue there is no entanglement) the state is separable but one or both of the quantum sub-systems violates the SSR. The sceptic may favor the second conclusion, but that would then imply an *actual* experimental circumstance where superselection rules did *not* apply to the sub-system states. In that case, the issues raised in the last four paragraphs regarding *lack* of *phase references* or SSR *violating preparation processes* etc must be addressed directly. Either way, the study of such SSR based experiments is clearly important. Put another way, suppose the sceptic were to derive a *different* test using the separability requirement *alone,* for which an experimental outcome shows that the two subsystems were indeed *not*entangled. This would seem to require a test for entanglement which is *necessary* as well as being sufficient—the latter alone being usually the case for entanglement tests. Such criteria and measurements are a challenge, but not impossible even though we have not met this challenge in these two papers. If the conclusion from the earlier SSR *based* experiment was *either* entanglement *or* separability with non-SSR compliance, then if the result from the different test based *only* on separability ruled entanglement *out*, it follows that the system must be in a separable state in which the sub-system states violate the SSR. Conversely, the latter test may confirm the entanglement possibility found in the earlier test. Thus, *in principle* there could be a *pair* of experiments that give evidence of entanglement, *or* failure of the Super Selection Rule. For such investigations to be possible, the use of entanglement criteria that *do* invoke the local SSRs is *also* required.

1.5. Entanglement tests and experiments—paper II

The main focus of the accompanying paper II [6] is to derive the SSR compliant criteria and to consider the experimental implementation. This leads to important links between *spin squeezing* and entanglement. The link with *quantum correlation functions* (as proposed in [61, 62]) is also treated. Heisenberg uncertainty principle (HUP) inequalities involving spin operators [72] 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* [73] 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 Sørensen *et al* [74], 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 Sørensen *et al* is often referred to as establishing the link between spin squeezing and entanglement—see for example Micheli *et al* [75], Toth *et al* [76], Hyllus *et al* [77]. However, the paper by Sørensen *et al* [74] 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. However, the accompanying paper II establishes the link between spin squeezing and entanglement based on a definition of entanglement consistent with the system and sub-system density operators representing quantum states.

It is also important to consider which *components* of the spin operator vector are squeezed, and this issue is also considered in the accompanying paper. In the context of the present second quantization 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 2 in the accompanying paper II) 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 also defined in terms of rotated spin operators referred to as *principal spin operators* for which the covariance matrix is *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 *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.

A further focus of the accompanying paper is on the relationship between entanglement and certain *correlation properties* of sub-system operators. Tests for entanglement based on such correlations have also been published—see for example [61, 62]. These tests were based on ignoring the SSRs, so in the accompanying paper we present revised correlation tests for entanglement when the SSRs are definitely complied with. We also show the link between correlation tests and tests involving spin operators.

The accompanying paper also deals with the important question of what *measurement systems* are suitable for making spin and correlation tests for entanglement. We first consider a *simple two mode interferometer* which involves coupling the two modes employing a *resonant classical field*

pulse which is associated with a variable *pulse area* for its amplitude and has an adjustable *phase*. It is shown that measurement of the mean value and variance of the *population difference* between the two modes *after* the interferometer pulse enables measurements of the *mean value* and *covariance matrix* elements of the *spin operators* for the quantum state that existed *before* the pulse was applied. The mean values and variances of certain spin operators are relevant for correlation and spin squeezing entanglement tests.

Paper II is focused on *two mode* systems of massive bosons. These are of particular interest because cold atomic gases cooled well below the Bose–Einstein condensation (BEC) transition temperature can be prepared where essentially only two modes are occupied [38, 78]. This can be achieved for cases involving a single hyperfine components using a double well trap potential or for two hyperfine components using a single well. At higher temperatures more than two modes may be occupied, so *multi-mode* systems are also of importance and thus are considered in paper II.

1.6. Outlines of papers I and II

The plan of the present paper is as follows. In section 2 the key definitions of entangled states are covered, and a detailed discussion on why the symmetrization principle and the SSR is invoked in discussed in section 3. The final section 4 summarizes and discusses the key features about entanglement treated in this paper. Details are in the appendices (stacks.iop.org/ps/92/023004/mmedia).

Challenges to the necessity of the SSR are outlined, with arguments against such challenges dealt with in appendices K and M. Two key mathematical inequalities are derived in appendix E and the Werner states (relevant to LHV theory) are defined in appendix A. LHV violations in the entangled GHZ state is discussed in appendix D. The proof of the Bell inequality is presented in appendix G. Classical entanglement is described in appendix B, and applying the SSRs for photons is discussed in appendix L. The concept of entanglement due to symmetrization and how this might be recognized is treated in appendix I. Details regarding the EPR paradoxes are given in appendix F. Detailed proofs relating to quantum correlations are given in appendices H and J. Mathematical expressions regarding conditional probabilities are set out in appendix C and criteria for local and global SSR are proven in appendix N.

In the accompanying paper II [6], section 2 sets out the definitions of spin squeezing and in the following section 3 it is shown that spin squeezing is a signature of entanglement, both for the original spin operators with entanglement of the original modes and the principle spin operators with entanglement of the two new modes, and also for multi-mode cases. Details of the latter are in appendices A and D. The significnce of the spin squeezing test is discussd in appendix C. A number of other tests for entanglement proposed by other authors are considered in sections 4–6, with details of these treatments set out in appendices E, F, G, H, I, J and L. In section 7 it is shown that a simple two mode interferometer can be used to measure the mean values and covariance matrix for the spin operators involved in entanglement tests. The treatment is then generalized to situations involving measurements on multi-mode systems. Details are covered in appendices M and N. Actual experiments aimed at detecting entanglement via spin squeezing tests are examined in section 8. The final section 9 summarizes and discusses the key results regarding entanglement tests. Appendices K and O provide details regarding certain important states whose features are discussed in the paper—the 'separable but non-local' states and the relative phase eigenstate.

2. Entanglement—general features

2.1. Quantum states

The standard Copenhagen quantum theory notions of *physical systems* that can exist in various *states* and have associated *properties* on which *measurements* can be made are presumed in this paper. The measuring system may 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 *quantum state* (or 'physical quantum state' or just 'state' for short) 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*). We may also refer to such states as *allowed* quantum states, and our approach is intended to be *physically* based. In quantum theory, quantum states are *represented* mathematically by *density operators* for mixed states or *state vectors* for pure states. For identical particle systems these representations must satisfy symmetrization and other basic requirements in accordance with the laws of quantum theory. The probabilities of measurement outcomes and the probabilities associated with retrodiction can be interpreted as *Bayesian probabilities* [79, 80], and the quantum state is *observer dependent.* The quantum state, the system it is associated with and the quantities that can be measured are considered here as entities that are viewed as being *both* ontological and epistemological. Different observers may have different information about how the quantum state was prepared, hence the quantum state is in part *epistemological*, and would be described differently by different observers. Hence the observer is important, but as there is actually something out there to be studied, quantum states also have an *ontological* aspect. We will avoid the unqualified term 'physical state' because this term is generally invoked in discussions about the pre-Copenhagen notion of *reality* and refers to some as yet unknown but more fundamental description of the system which underlies the quantum state [81]. HVTs attempt to describe this more fundamental physical state that is assumed to exist—attempts that so far have been unsuccessful if locality is also invoked (see below). In addition to those associated with physical quantum states,

other density operators and state vectors may be introduced for mathematical convenience. For physical quantum states, the density operator is determined from either the preparation process or inferred from the measurement process—*quantum tomography*—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 quantum 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* [79, 82]. While there are often different mathematical forms for the density operator that lead to the same predictive results for subsequent measurements, the results of the measurements can also be used to retrodictively determine the *preferred form* of the density operator that is consistent with the available preparation and measurement operators. An example is given in [82].

2.2. Entangled and non-entangled states

2.2.1. General considerations. Here the commonly applied *physically based approach* to mathematically defining entangled states will be described [18]. The definition involves vectors and density operators that represent states than can be prepared in real experiments, so the mathematical approach is to be *physically based*. The concept of quantum entanglement involves *composite systems* made up of component *sub-systems* each of which are *distinguishable* from the other sub-systems, and where each could constitute a stand-alone quantum system. This means the each sub-system will have its own set of physically realizable quantum states —mixed or pure—which could be prepared independently of the quantum states of the other sub-systems. As will be seen, the requirement that sub-systems be distinguishable and their states be physically preparable will have important consequences, especially in the context of identical particle systems. 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 allows for *pure states* for composite systems made up of two or more distinct sub-systems via tensor products of sub-system states

$$|\Phi\rangle = |\Phi_A\rangle \otimes |\Phi_B\rangle \otimes |\Phi_C\rangle .... \tag{1}$$

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

$$|\Phi\rangle = \sum_{\alpha\beta\gamma..} C_{\alpha\beta\gamma..} |\Phi_A^{\alpha}\rangle \otimes |\Phi_B^{\beta}\rangle \otimes |\Phi_C^{\gamma}\rangle ... \tag{2}$$

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, ... are the sub-systems with $\hat{\rho}_R^A$, $\hat{\rho}_R^B$, being density operators the sub-systems A, B, 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 [7]

$$\hat{\rho} = \sum_R P_R \, \hat{\rho}_R^A \otimes \hat{\rho}_R^B \otimes \hat{\rho}_R^C \otimes ... \tag{3}$$

with $\sum_R P_R = 1$ and $P_R \geqslant 0$ giving the probability that the specific product state $\hat{\rho}_R = \hat{\rho}_R^A \otimes \hat{\rho}_R^B \otimes \hat{\rho}_R^C \otimes ...$ occurs. It is assumed that at least in principle such separable states can be prepared [7]. This implies the possibility of turning off the interactions between the different sub-systems, a task that may be difficult in practice except for well-separated sub-systems. *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 density operator $\hat{\rho} = |\Phi\rangle\langle\Phi|$ for the pure state in (2) is not of the form (3), as there are cross terms of the form $C_{\alpha\beta\gamma..} C^*_{\theta\lambda\eta..} (|\Phi_A^{\alpha}\rangle\langle\Phi_A^{\theta}|) \otimes (|\Phi_B^{\beta}\rangle\langle\Phi_B^{\lambda}|) \otimes ...$ involved.

The concepts of separability and entanglement based on the equations (1) and (3) for non-entangled states do not however just rest on the mathematical forms alone. Implicitly there is the *assumption* that separable quantum states described by the two expressions can actually be created in *physical processes*. The sub-systems involved must therefore be *distinguishable quantum systems* in their own right, and the sub-system states $|\Phi_A\rangle$, $|\Phi_B\rangle$, ... or $\hat{\rho}_R^A$, $\hat{\rho}_R^B$, ... must also be *possible quantum states* for the sub-systems. We will return to these requirements later. The issue of the physical preparation of non-entangled (separable) states starting from some uncorrelated fiducial state for the separate sub-systems was introduced by Werner [7], and discussed further by Bartlett *et al* (see [54], section IIB). This involves the ideas of LOCC dealt with in the next section.

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 $\hat{\rho}_R^A$, $\hat{\rho}_R^B$, etc and the overall classical probability P_R (see section 2.3). This feature of separable probabilities is absent in *certain* 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 HVTs (see section 2.5) applied to quantum systems—as well as to quantum separable states. The fact that entangled states are quantum states that can exhibit the failure of this separability feature for classical LHV theories highlights entanglement being a non-classical feature for 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 [36, 47], and a *utilitarian approach* focuses or whether entangled states have technological applications such as in various quantum information protocols. As will be seen in section 3.4, the particular definition of entangled states based on their non-creatability via LOCC essentially coincides with the approach used in the present paper. It has been realized for some time that different types of entangled states occur, for example states in which a Bell inequality is *not* violated or states demonstrating an EPR paradox [83]. Wiseman *et al* [27–29] and Reid *et al* [19, 20, 30, 84] discuss the concept of a *hierarchy* of *entangled states*, with states exhibiting *Bell non-locality* being a subset of states for which there is EPR *steering*, which in turn is a subset of all the *entangled states*, the latter being defined as states whose density operators cannot be written as in equation (3) 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 physical approach based on the quantities involved representing allowed sub-system states is generally favored [18]. It is also compatible with later classifying entangled states in a hierarchy.

Finally, we should mention that in addition to quantum entanglement, there is a body of work dealing with so-called classical entanglement. This is essentially of mathematical rather than physical interest, but for completeness a brief summary is presented in appendix B.

2.2.2. Local systems and operations. As pointed out by Vedral [17], one reason for calling states such as in equations (1) and (3) 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 $\widehat{U}_A$, $\widehat{U}_B$, that change the states via $\widehat{\rho}_R^A \rightarrow \widehat{U}_A \widehat{\rho}_R^A \widehat{U}_A^{-1}$, $\widehat{\rho}_R^B \rightarrow \widehat{U}_B \widehat{\rho}_R^B \widehat{U}_B^{-1}$, etc as in a time evolution, and could include processes by which the states $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, 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 *localized*. As described by Werner [7], if one observer (Alice) is associated with preparing separate sub-system A in an allowed quantum state $\widehat{\rho}_R^A$ 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 $\widehat{\rho}_R^B$ 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 $\widehat{\rho} = \sum_R P_R \widehat{\rho}_R^A \otimes \widehat{\rho}_R^B$. Multipartite non-entangled states of the form (3) 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 $\widehat{\rho}$ and $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, in equation (3) always represent possible *quantum states*, even if the operators $\widehat{\rho}$ and $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, etc satisfy all the standard mathematical requirements for density operators—Hermitiancy, positiveness, trace equal to unity, trace of density operator squared being not greater than unity. In this paper it will be argued that for systems of identical massive particles there are further requirements not only on the overall density operator, but also (for separable states) on those for the individual sub-systems that are imposed by *symmetrization* and SSRs.

2.3. Separate and joint measurements, reduced density operator

In this section 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 $\widehat{\Omega}$, which project the quantum state into subspaces for the eigenvalue λ_i that is measured, the subspaces being associated with Hermitian, idempotent *projectors* $\widehat{\Pi}_i$ whose sum over all eigenvalues is unity. These concepts are treated in several quantum theory textbooks, for example [15, 85]. For completeness, an account setting out the key results is presented in appendix C.

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 $\widehat{\Omega}_A$ is a physical quantity associated with sub-system A, with eigenvalues λ_i^A and with $\widehat{\Pi}_i^A$ the projector onto the subspace with eigenvalue λ_i^A, $\widehat{\Omega}_B$ is a physical quantity associated with sub-system B, with eigenvalues λ_j^B and with $\widehat{\Pi}_j^B$ the projector onto the subspace with eigenvalue λ_j^B etc, then the *joint*

probability $P_{AB..}(i, j, \ldots)$ that measurement of $\widehat{\Omega}_A$ leads to result λ_i^A, measurement of $\widehat{\Omega}_B$ leads to result λ_j^B, etc is given by

$$P_{AB..}(i, j, \ldots) = \mathrm{Tr}(\widehat{\Pi}_i^A \, \widehat{\Pi}_j^B \ \ldots \ \widehat{\rho}). \tag{4}$$

This joint probability depends on the full density operator $\widehat{\rho}$ representing the allowed quantum state as well as on the quantities being measured. Here the projectors (strictly $\widehat{\Pi}_i^A \otimes \hat{1}^B \otimes \ldots$, $\hat{1}^A \otimes \widehat{\Pi}_j^B \otimes \ldots$, etc) commute, so the order of measurements is immaterial. An alternative notation in which the physical quantities are also specified is $P_{AB..}(\widehat{\Omega}_A, i; \widehat{\Omega}_B, j; \ldots)$.

2.3.2. Single measurements on sub-systems and reduced density operator. The *reduced density operator* $\widehat{\rho}_A$ for sub-system A given by

$$\widehat{\rho}_A = \mathrm{Tr}_{B,C,\ldots}(\widehat{\rho}) \tag{5}$$

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 $\widehat{\Omega}_A$ leads to result λ_i^A irrespective of the results for measurements on the other sub-systems is given by

$$\begin{aligned} P_A(i) &= \sum_{j,k,\ldots} P_{AB..}(i, j, \ldots) \\ &= \mathrm{Tr}(\widehat{\Pi}_i^A \, \widehat{\rho}) \qquad (6) \\ &= \mathrm{Tr}_A(\widehat{\Pi}_i^A \, \widehat{\rho}_A) \qquad (7) \end{aligned}$$

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

2.3.3. Mean value and variance. The *mean value* for measuring a physical quantity $\widehat{\Omega}_A$ will be given by

$$\begin{aligned} \langle \widehat{\Omega}_A \rangle &= \sum_{\lambda_i^A} \lambda_i^A P_A(i) \\ &= \mathrm{Tr}_A(\widehat{\Omega}^A \, \widehat{\rho}_A), \end{aligned} \tag{8}$$

where we have used $\widehat{\Omega}^A = \sum_{\lambda_i^A} \lambda_i^A \widehat{\Pi}_i^A$.

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

$$\begin{aligned} \langle (\Delta\widehat{\Omega}^A)^2 \rangle &= \sum_{\lambda_i^A} (\lambda_i^A - \langle \widehat{\Omega}_A \rangle)^2 P_A(i) \\ &= Tr_A((\widehat{\Omega}^A - \langle \widehat{\Omega}_A \rangle)^2 \, \widehat{\rho}_A) \end{aligned} \tag{9}$$

so both the mean and variance only depend on the reduced density operator $\widehat{\rho}_A$.

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

$$\begin{aligned} \langle \widehat{\Omega}_A \otimes \widehat{\Omega}_B \otimes \widehat{\Omega}_C \otimes . \rangle &= \sum_{\lambda_i^A} \sum_{\lambda_j^B} \ldots \lambda_i^A \lambda_j^B \ldots P_{AB..}(i, j, \ldots) \\ &= Tr(\widehat{\Omega}_A \otimes \widehat{\Omega}_B \otimes \widehat{\Omega}_C \otimes .)\widehat{\rho} \end{aligned} \tag{10}$$

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 C, equation (103)) to obtain expressions for *conditional probabilities* [18]. The conditional probability that if measurement of $\widehat{\Omega}_B$ associated with sub-system B leads to eigenvalue λ_j^B then measurement of $\widehat{\Omega}_A$ associated with sub-system A leads to eigenvalue λ_i^A is given by

$$P_{AB}(i|j) = \mathrm{Tr}(\widehat{\Pi}_i^A \, \widehat{\Pi}_j^B \, \widehat{\rho}) / \mathrm{Tr}(\widehat{\Pi}_j^B \widehat{\rho}). \tag{11}$$

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 $P_{AB}(\widehat{\Omega}_A, i|\widehat{\Omega}_B, j)$.

As shown in appendix C the conditional probability is given by

$$P_{AB}(i|j) = \mathrm{Tr}(\widehat{\Pi}_i^A \, \widehat{\rho}_{\mathrm{cond}}(\widehat{\Omega}_B, \lambda_j^B)), \tag{12}$$

where

$$\widehat{\rho}_{\mathrm{cond}}(\widehat{\Omega}_B, \lambda_j^B) = \widehat{\Pi}_j^B \, \widehat{\rho} \, \widehat{\Pi}_j^B / \mathrm{Tr}(\widehat{\Pi}_j^B \widehat{\rho}) \tag{13}$$

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

$$P_{AB}(i|j) = \mathrm{Tr}(\widehat{\Pi}_i^A \widehat{\rho}_{\mathrm{cond}}(\widehat{\Omega}_B, \lambda_j^B)) \tag{14}$$

which is the same as the expression (6) with $\widehat{\rho}$ replaced by $\widehat{\rho}_{\mathrm{cond}}(\widehat{\Omega}_B, \lambda_j^B)$. This is what would be expected for a conditioned measurement probability.

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

$$\begin{aligned} \widehat{\rho}_{\mathrm{cond}}(\widehat{\Omega}_B) &= \sum_{\lambda_j^B} P_B(j) \widehat{\rho}_{\mathrm{cond}}(\widehat{\Omega}_B, \lambda_j^B) \\ &= \sum_{\lambda_j^B} \widehat{\Pi}_j^B \, \widehat{\rho} \, \widehat{\Pi}_j^B. \end{aligned} \tag{15}$$

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

$$\begin{aligned} P_{AB}(i|Any\ j) &= \mathrm{Tr}(\widehat{\Pi}_i^A \widehat{\rho}_{\mathrm{cond}}(\widehat{\Omega}_B)) \\ &= \mathrm{Tr}(\widehat{\Pi}_i^A \widehat{\rho}) \qquad (16) \\ &= P_A(i), \qquad (17) \end{aligned}$$

where we have used the cyclic properties of the trace, $(\widehat{\Pi}_j^B)^2 = \widehat{\Pi}_j^B$ and $\sum_{\lambda_j^B} \widehat{\Pi}_j^B = \hat{1}$. The results in equations (16) and (17) are the same as the measurement probability for $\widehat{\Omega}_A$ if no measurement for $\widehat{\Omega}_B$ 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 that $\sum_j P_{AB}(i|j)P_B(j) = \sum_j P_{AB}(i, j) = P_A(i)$, since $\sum_j P_{AB}(i, j)$ is the probability that measurement of $\widehat{\Omega}_A$ will lead to λ_i^A and measurement of $\widehat{\Omega}_B$ will lead to any of the λ_j^B. This result is called the no-signalling theorem [18].

Also, as $P_{AB}(i|Any\ j) = \mathrm{Tr}(\widehat{\Pi}_i^A \hat{\rho}_{\mathrm{cond}}(\widehat{\Omega}_B))$ we see from (7) that

$$\hat{\rho}_A = \mathrm{Tr}_B(\hat{\rho}_{\mathrm{cond}}(\widehat{\Omega}_B)) \tag{18}$$

showing that the trace over B of the conditioned density operator for the state obtained by measuring *any* observable $\widehat{\Omega}_A$ and then discarding the results just gives the *reduced density operator* for sub-system A.

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

$$\begin{aligned}\langle\widehat{\Lambda}\rangle_{\widehat{\Omega},i} &= \mathrm{Tr}(\widehat{\Lambda}\hat{\rho}_{\mathrm{cond}}(\widehat{\Omega}, i)) \\ &= \sum_j \mu_j\, P(\widehat{\Lambda}, j|\widehat{\Omega}, i).\end{aligned} \tag{19}$$

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

$$\begin{aligned}\langle\Delta\widehat{\Lambda}^2\rangle_{\widehat{\Omega},i} &= Tr((\widehat{\Lambda} - \langle\widehat{\Lambda}\rangle_{\widehat{\Omega},i})^2\hat{\rho}_{\mathrm{cond}}(\widehat{\Omega}, i)) \\ &= \sum_j (\mu_j - \langle\widehat{\Lambda}\rangle_{\widehat{\Omega},i})^2\, P(\widehat{\Lambda}, j|\widehat{\Omega}, i).\end{aligned} \tag{20}$$

If we weighted the conditioned mean by the probability $P(\widehat{\Omega}, i)$ that measuring $\widehat{\Omega}$ has led to the eigenvalue λ_i and summed over the possible outcomes λ_i for the $\widehat{\Omega}$ measurement, then we obtain the mean for measurements of $\widehat{\Lambda}$ after unrecorded measurements of $\widehat{\Omega}$ have occurred. From Bayes theorem $\sum_i P(\widehat{\Lambda}, j|\widehat{\Omega}, i)P(\widehat{\Omega}, i) = P(\widehat{\Lambda}, j)$ so this gives the *unrecorded mean* $\langle\widehat{\Lambda}\rangle_{\widehat{\Omega}}$ as

$$\begin{aligned}\langle\widehat{\Lambda}\rangle_{\widehat{\Omega}} &= \sum_i \langle\widehat{\Lambda}\rangle_{\widehat{\Omega},i} P(\widehat{\Omega}, i) \\ &= \sum_j \mu_j\, P(\widehat{\Lambda}, j) \\ &= \langle\widehat{\Lambda}\rangle\end{aligned} \tag{21}$$

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

$$\begin{aligned}\langle\Delta\widehat{\Lambda}^2\rangle_{\widehat{\Omega}} &= \sum_i \langle\Delta\widehat{\Lambda}^2\rangle_{\widehat{\Omega},i} P(\widehat{\Omega}, i) \\ &\neq \langle\Delta\widehat{\Lambda}^2\rangle.\end{aligned} \tag{22}$$

2.4. Non-entangled states

In this section 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

$$P_{AB..}(i, j, \ldots) = \sum_R P_R\, P_A^R(i) P_B^R(j)\ \ldots\ , \tag{23}$$

where

$$P_A^R(i) = Tr(\widehat{\Pi}_i^A\, \hat{\rho}_R^A) \qquad P_B^R(j) = Tr(\widehat{\Pi}_j^B\, \hat{\rho}_R^B).. \tag{24}$$

are the probabilities for measurement results for $\widehat{\Omega}_A$, $\widehat{\Omega}_B$, ... 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 $P_A^R(i)$, $P_B^R(j)$, .. for the measurement results λ_i^A, λ_j^B, ... for physical quantities $\widehat{\Omega}_A$, $\widehat{\Omega}_B$, ... if the sub-systems are in the states $\hat{\rho}_R^A$, $\hat{\rho}_R^B$, etc. Note that here $P_A^R(i)$, $P_B^R(j)$, are given by quantum theory formulae for the subsystem states. For simplicity only quantized measured values will be considered—the extension to continuous values is straightforward. Thus the results for the probabilities of joint measurements when the system is in a separable quantum state are determined by the measurement probabilities in *possible* quantum states for the sub-systems, combined with a *classical* probability for creating the particular set of sub-system quantum states. Note the emphasis on 'possible'—some of the separable states described in [56] are not possible.

Furthermore, if we consider measurements of the physical quantity $\widehat{\Omega}_A \otimes \widehat{\Omega}_B$ then for a separable state the *mean value* for measurement of this quantity is given by

$$\langle\widehat{\Omega}_A \otimes \widehat{\Omega}_B\rangle = \mathrm{Tr}(\widehat{\Omega}_A \otimes \widehat{\Omega}_B\, \hat{\rho}) = \sum_R P_R \langle\widehat{\Omega}_A\rangle_R^A \langle\widehat{\Omega}_B\rangle_R^B\ , \tag{25}$$

where $\langle\widehat{\Omega}_A\rangle_R^A = \mathrm{Tr}_a(\widehat{\Omega}_A\, \hat{\rho}_R^A)$ and $\langle\widehat{\Omega}_B\rangle_R^B = \mathrm{Tr}_b(\widehat{\Omega}_B\, \hat{\rho}_R^B)$ are the mean values of $\widehat{\Omega}_A$ and $\widehat{\Omega}_B$ for the sub-system states $\hat{\rho}_R^A$ and $\hat{\rho}_R^B$ respectively. If $\langle\widehat{\Omega}_A \otimes \widehat{\Omega}_B\rangle = \langle\widehat{\Omega}_A\rangle\langle\widehat{\Omega}_B\rangle$ then the state is said to be *uncorrelated*. Separable states are *correlated* except for the case where $\hat{\rho}_{\mathrm{sep}} = \hat{\rho}^A \otimes \hat{\rho}^B$, but the correlation is essentially *non-quantum* and attributable to the classical probabilities P_R. However, for separable states the inequality $|\langle\widehat{\Omega}_A \otimes \widehat{\Omega}_B^\dagger\rangle|^2 \leqslant \langle\widehat{\Omega}_A^\dagger\widehat{\Omega}_A \otimes \widehat{\Omega}_B^\dagger\widehat{\Omega}_B\rangle$ applies, so that if $|\langle\widehat{\Omega}_A \otimes \widehat{\Omega}_B^\dagger\rangle|^2 > \langle\widehat{\Omega}_A^\dagger\widehat{\Omega}_A \otimes \widehat{\Omega}_A^\dagger\widehat{\Omega}_A\rangle$ then the state is entangled.

In the simple non-entangled *pure state* situation in equation (1) the joint probability only involves a single

product of sub-system probabilities

$$P_{AB..}(i, j, \ ...) = P_A(i)P_B(j)..., \tag{26}$$

where

$$P_A(i) = \langle\Phi_A|\widehat{\Pi}_i^A|\Phi_A\rangle \quad P_B(j) = \langle\Phi_B|\widehat{\Pi}_j^B|\Phi_B\rangle \ .. \tag{27}$$

just give the probabilities for measurements in the separate sub-systems.

This *key result* (23) 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* necessarily apply for entangled states [7]. However the *key quantum feature* for *composite systems* of non-separability for joint measurement probabilities applies only to entangled states. This strange quantum feature of entangled states has been regarded as particularly unusual when the sub-systems are *spatially well-separated* (or non-local) because then measurement events can become space-like separated. This is relevant to quantum paradoxes such as Einstein–Poldolsky–Rosen and Bell's theorem which aim to show there could be no causal classical theory explaining quantum mechanics [1, 2]. Measurements on sub-system A of physical quantity $\widehat{\Omega}_A$ affect the results of measurements of $\widehat{\Omega}_B$ at the same time on a distant sub-system B, even if the choice of measured quantity $\widehat{\Omega}_B$ is unknown to the experimenter measuring $\widehat{\Omega}_A$. As will be shown below, a similar result to (23) also occurs in HVT—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 sub-system measurements. For the general non-entangled state, the reduced density operator for sub-system A is given by

$$\widehat{\rho}_A = \sum_R P_R \ \widehat{\rho}_R^A. \tag{28}$$

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* subsystems. From equations (7) and (28) the probability $P_A(i)$ that measurement of $\widehat{\Omega}_A$ leads to result λ_i^A is given by

$$P_A(i) = \sum_R P_R \ P_A^R(i), \tag{29}$$

where the reduced density operator is given by equation (28) for the non-entangled state in equation (3). This result only depends on the reduced density operator $\widehat{\rho}_A$, which represents a state for sub-system A and which is a statistical mixture of the sub-system states $\widehat{\rho}_R^A$, 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 $\widehat{\rho}_R^A$. For all quantum states the final expression for the measurement probability $P_A(i)$ only involves a trace of quantities $\widehat{\Pi}_i^A$, $\widehat{\rho}_A$ that apply to sub-system A, but for a non-entangled state the reduced density operator $\widehat{\rho}_A$ is given by an expression (28) 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 $\widehat{\rho}_R^B$, $\widehat{\rho}_R^C$, 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

$$P_{AB}(i|j) = \sum_R P_R \ P_A^R(i)P_B^R(j)/\sum_R P_R P_B^R(j) \tag{30}$$

which in general depends on $\widehat{\Omega}_B$ associated with sub-system B and the eigenvalue λ_j^B. This may seem surprising for the case where A and B are localized sub-systems which are well separated. Even for separable states a measurement result for sub-system B will give *immediate* information about a totally separated measurement on sub-system A—which is *space-like* separated. However it should be remembered that the general separable system can still be a *correlated* state, since each sub-system density operator $\widehat{\rho}_R^B$ for sub-system B is matched with a corresponding density operator $\widehat{\rho}_R^A$ for sub-system A. Results at A can be correlated with those at B, so the observer at A can potentially infer from a local measurement on the sub-system A the result of a local measurement on sub-system B. It is therefore not necessarily the case that measurement results for A are independent of those for B. However, as we will see below, such correlations (usually) have a classical interpretation. Result (30) is *not* a case of the 'spooky action at a distance' that Einstein [1] referred to.

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

$$P_{AB}(i|j) = P_A(i), \tag{31}$$

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

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 $\widehat{\Omega}_B$ are discarded then the probability distribution for measurements on $\widehat{\Omega}_A$ will be determined from the conditioned density operator $\widehat{\rho}_{\mathrm{cond}}(\widehat{\Omega}_B)$ and just result in $P_A(i)$—as in shown in equation (17) for any quantum state.

2.4.4. Non-entangled states—mean values and correlations. For non-entangled states as in equation (3) the mean value for measuring a physical quantity $\widehat{\Omega}_A \otimes \widehat{\Omega}_B \otimes \widehat{\Omega}_C \otimes ...$, where $\widehat{\Omega}_A$, $\widehat{\Omega}_B$, $\widehat{\Omega}_C$, .. are Hermitian operators representing physical quantities for the separate sub-systems can be obtained from equations (3) and (10), and is given by

$$\langle\widehat{\Omega}_A \otimes \widehat{\Omega}_B \otimes \widehat{\Omega}_C \otimes .\rangle = \sum_R P_R \langle\widehat{\Omega}_A\rangle_R^A \langle\widehat{\Omega}_B\rangle_R^B \langle\widehat{\Omega}_C\rangle_R^C..., \tag{32}$$

where

$$\langle\widehat{\Omega}_K\rangle_R^K = Tr(\widehat{\Omega}_K \ \widehat{\rho}_R^K), \quad (K = A, B, \ ...) \tag{33}$$

is the mean value for measuring $\widehat{\Omega}_K$ in the K sub-system when

its density operator is $\widehat{\rho}_R^K$. 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* [18]. In the case of a single product state where $\widehat{\rho} = \widehat{\rho}^A \otimes \widehat{\rho}^B \otimes \widehat{\rho}^C \otimes ...$ we have $\langle \widehat{\Omega}_A \otimes \widehat{\Omega}_B \otimes \widehat{\Omega}_C \otimes ... \rangle = \langle \widehat{\Omega}_A \rangle^A \langle \widehat{\Omega}_B \rangle^B \langle \widehat{\Omega}_C \rangle^C ...$ 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 $\langle \widehat{\Omega}_A \otimes \widehat{\Omega}_B \otimes \widehat{\Omega}_C \otimes ... \rangle$ does not apply, and the correlation is strictly quantum.

2.5. LHV theories

In a general LHV *theory* as envisaged by Einstein *et al* [1] and Bell [4], physical quantities associated with the sub-systems are denoted Ω_A, Ω_B etc, which are real numbers not operators. Their values are assumed to be λ_i^A, λ_j^B etc—having the same ranges 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, the probabilities for measuring these values being determined from a set of hidden variables ξ, which are themselves given by a probability function $P(\xi)$ for each state preparation process. Measurement is *not* required for the values for physical quantities to be created, as in quantum theory, nor do the hidden variables change as a result of the act of measurement itself (though they may change as a result of local interactions of the system with the measurement apparatus [86, 87]. As in classical physics, ideal measurement is assumed *not* to change the state of the system—the hidden variables would only change in accord with the (as yet unknown) dynamical equations that govern their evolution. The hidden variables are regarded as the *elements of reality* that constitute the fundamental way of describing the system [1]. There may be just a single hidden variable or a set, and the hidden variables could be discrete or continuous—these details do not matter in a general HVT. In the original treatment of Bell [4] the hidden variables uniquely determine the *actual* values that physical quantities would have when measured. However, in a so-called '*fuzzy*' HVT [9, 19, 86–89] (see also section 7.1 of [17]) the values for Ω_A, Ω_B etc are determined *probabilisticly* from the hidden variables, the probability functions being *classical* and allow for the hidden variables not being known—just as in classical statistical mechanics, where the unknown (but real) positions and momenta of the classical particles are described via probabilities. The probabilistic treatment of the hidden variables attempts to replicate the probabilistic nature of quantum theory. For our purposes we will consider only LHV theories —this is sufficient to demonstrate key results such as the Bell inequalities. For LHV theories although the hidden variables ξ are *global*, they act locally even for spatially separable sub-systems. For particular hidden variables ξ the probability that Ω_A has value λ_i^A will be given by $P_A(i, \xi)$ and the probability that Ω_B has value λ_j^B will be given by $P_B(j, \xi)$, etc. The LHVT joint probability for measurement outcome for Ω_A, Ω_B, etc will be given by

$$P_{AB..}(i, j, ..) = \int \mathrm{d}\xi \, P(\xi) P_A(i, \xi) P_B(j, \xi) .... \tag{34}$$

States where the joint probabilities are given by (34) are the *Bell local* states, all other states are *Bell non-local*. Here $P(\xi)\mathrm{d}\xi$ is the probability that the hidden variables are in the range $\mathrm{d}\xi$ around ξ, the HV being assumed continuous—which is not a requirement [4]. The probabilities satisfy the usual sum rules for all outcomes giving unity, thus $\sum_i P_A(i, \xi) = 1$, etc, $\int \mathrm{d}\xi P(\xi) = 1$. The sub-system probabilities $P_A(i, \xi)$, $P_B(j, \xi)$ etc only depend on the hidden variables ξ. Bell inequalities are constraints derived on the basis of the assumption (34), and if violated therefore falsify all LHV theories. The Bell inequalities will be discussed further in section 2.7.

The *formal similarity* between the HVT expression for the joint probability (34) and the quantum expression (23) for a separable state is noticeable. We could map $\xi \to R$, $P(\xi) \to P_R$, $\int \mathrm{d}\xi \Rightarrow \sum_R$, $P_A(i, \xi) \to P_A^R(i)$ and $P_B(j, \xi) \to P_B^R(j)$. The Werner preparation process [7] would then determine the setting for the hidden variables ξ. If a HVT *underpinned* quantum theory, it follows that the quantum probabilities $P_A^R(i)$ and $P_B^R(j)$ would always be equivalent to hidden variable probabilities $P_A(i, \xi)$ or $P_B(j, \xi)$ for each of the sub-systems (it would not be consistent to only have this apply to one of the sub-systems and not the other). Thus, all *separable* states are Bell local. From the expression (34) for the joint probability general HVT expressions for the mean value $\langle \Omega_A \times \Omega_B \rangle_{\mathrm{HVT}}$ for the product of the measurement results for observables Ω_A and Ω_B for subsystems A, B respectively (see (36) below) can be obtained that are analogous to the quantum expression (32) for a separable state. There is of course no independent fully developed classical HVT that can actually predict the $P_A(i, \xi)$, $P_B(j, \xi)$ etc.

However, as we will see both the HVT (see [18] for a proof) and the quantum separable state predictions are consistent with Bell Inequalities, and it therefore requires a quantum entangled state to violate Bell inequalities and to demonstrate failure of the LHV theory model (34). Naturally it follows that such quantum entangled states cannot be described via a LHV theory. Hence the *experimental violation* of Bell inequalities would *also* show that the particular quantum state must be *entangled*. Note however that as Werner [7] showed, some entangled states are also Bell local, so although all Bell non-local states are entangled, not all entangled states are Bell non-local (see [27–29]).

A clear example of an entangled quantum state which cannot be described via LHV theory [90–92] is the GHZ state. This involves three sub-systems each with two basis states and measurements involving Pauli spin operators. A discussion of LHV violation in the GHZ state is included for completeness in appendix D.

2.5.1. LHV—mean values and correlation. The actual values that would be assigned to the physical quantities Ω_A, Ω_B etc will depend on the hidden variables but can be taken as the *mean values* of the possible values λ_i^A, λ_i^A etc. We denote these mean values as $\langle\Omega_A(\xi)\rangle$, $\langle\Omega_B(\xi)\rangle$ etc where

$$\langle\Omega_K(\xi)\rangle = \sum_{\lambda_k^K} \lambda_k^K P_K(k, \xi) \quad (K = A, B, \ldots). \tag{35}$$

These expressions my be compared to equation (33) for the mean values of physical quantities $\widehat{\Omega}_A$, $\widehat{\Omega}_B$ etc in quantum separable states.

We can then obtain an expression for the mean value in HVT of the physical quantity $\Omega_A \times \Omega_B \times \Omega_C \times ...$, where Ω_A, Ω_B, etc are physical quantities for the separate subsystems. This is obtained from equations (34) and (35) and is given by

$$\langle\Omega_A \times \Omega_B \times \Omega_C \times .\rangle_{\mathrm{LHV}} = \int \mathrm{d}\xi\, P(\xi)\langle\Omega_A(\xi)\rangle\langle\Omega_B(\xi)\rangle\langle\Omega_C(\xi)\rangle \ldots \tag{36}$$

This may be compared to equation (32) for the mean value of the physical quantity $\widehat{\Omega}_A \otimes \widehat{\Omega}_B \otimes \widehat{\Omega}_C \otimes ..$ in quantum separable states.

2.6. Paradoxes

The EPR and Schrödinger 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 any measurement is only known in terms of 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.

While the EPR and Schrödinger 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 section 2.7) 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 HVTs. It then became possible to carry out actual experiments to distinguish these two fundamentally different theories. The actual experimental evidence is consistent with quantum theory and (apart from a small number of remaining loopholes) rules out LHV theories.

2.6.1. EPR paradox. In the original version of the EPR paradox, Einstein *et al* [1] 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 $|\Phi\rangle$ of the two commuting operators $\hat{x}_A - \hat{x}_B$ and $\hat{p}_A + \hat{p}_B$, where $(\hat{x}_A - \hat{x}_B)|\Phi\rangle = 2x|\Phi\rangle$ and $(\hat{p}_A + \hat{p}_B)|\Phi\rangle = 0|\Phi\rangle$. This state is an example of an entangled state, as may be seen if it is expanded in terms of position eigenstates $|x_A x_B\rangle$. If the system is in state $|\Phi\rangle$ then from standard quantum theory 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 so that the two particles will be well-separated (in quantum theory their spatial wave functions would be localized in separate spatial regions) it follows 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. On the other hand, 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, so all these measurements do is reveal these (hidden) values. It would seem then that measurements of position and momentum on particle B *could* lead to a knowledge of the position and momentum at a far distant particle A, perhaps with an accuracy that would violate the HUP. As we will see, this is not the case when quantum theory is applied correctly. However, what Einstein *et al* pointed out as being particularly strange was that the choice of whether the momentum or position of B was measured (and found to have a definite value) would instantly determine which of the position or momentum of A would then have a definite value—even if A and B were separated by such a large distance that no signal could have been passed from B to A regarding which quantity was measured. Einstein referred to this as 'spooky action at a distance' to highlight the strangeness of what came to be referred to as entangled states. 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.

The EPR argument assumes *local realism*, to justify that the possibility of an exact *prediction* of the position of the far-away particle A (based on the measurement of the position for the particle B) implies the realist viewpoint that the position of particle A was predetermined. The same argument applies to the momentum of particle A, and hence EPR conclude that *both* the position and momentum of particle A are precisely predetermined—in conflict with the HUP derived from quantum mechanics. Since the argument is based on the assumption of local realism, the modern interpretation of the EPR analysis is that it reveals (for the appropriate entangled state) the inconsistency of local realism with the completeness of quantum mechanics.

Discussions of the EPR paradox [1] in terms of HVTs has been given by numerous authors (see [17–19, 89] for example). The papers and reviews by Reid *et al* [19, 83, 89], give a full account taking into consideration the 'fuzzy'

version of *local* HVT (LHV) and determining the predictions for the conditional variances for x_A and p_A based both on separable quantum states and states described via local 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 $\widehat{\rho}$ for the two particle system is changed into the conditional density operator $\widehat{\rho}_{\rm cond}(\widehat{x}_B, x) = \widehat{\Pi}_x^B \widehat{\rho}\, \widehat{\Pi}_x^B / {\rm Tr}(\widehat{\Pi}_x^B \widehat{\rho})$, where $\widehat{\Pi}_x^B = (|x\rangle\langle x|)_B$ 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 $\widehat{\rho}$ for the two particle system is changed into the conditional density operator $\widehat{\rho}_{\rm cond}(\widehat{p}_B, p) = \widehat{\Pi}_p^B \widehat{\rho}\, \widehat{\Pi}_p^B / {\rm Tr}(\widehat{\Pi}_p^B \widehat{\rho})$, where $\widehat{\Pi}_p^B = (|p\rangle\langle p|)_B$ 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. Conditional variances for position and momentum for sub-system A are considered based on measurements for sub-system B of position. It can be shown that for these conditional variances the HUP still applies. The same conclusion is obtained if the measurements on sub-system B had been the momentum. As the experimenter on sub-system A could not know whether the measurement on sub-system B was on position or momentum, the action at a distance feature of quantum entanglement is confirmed.

The question is whether the conditional variances $\langle \Delta \widehat{x}_A^2 \rangle_{\widehat{x}_B}$ for measuring $\widehat{x}_A$ for sub-system A having measured $\widehat{x}_B$ for sub-system B, and $\langle \Delta \widehat{p}_A^2 \rangle_{\widehat{p}_B}$ for measuring $\widehat{p}_A$ for sub-system A having measured $\widehat{p}_B$ for sub-system B violate the HUP [83]

$$\langle \Delta \widehat{x}_A^2 \rangle_{\widehat{x}_B} \langle \Delta \widehat{p}_A^2 \rangle_{\widehat{p}_B} < \frac{1}{4}\hbar^2, \tag{37}$$

where the measurements on sub-system B are left unrecorded. If this inequality holds we have an EPR *violation*. However for separable states it can be shown that $\langle \Delta \widehat{x}_A^2 \rangle_{\widehat{x}_B} \langle \Delta \widehat{p}_A^2 \rangle_{\widehat{p}_B} \geqslant \frac{1}{4}\hbar^2$. The proof of this result is set out in appendix F. Thus if the EPR violations as defined in equation (37) are to occur then the state must be entangled. Progress towards experimental confirmation of EPR violations is reviewed in [9, 19].

In [89] an analogous treatment based on LHV *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 LHV theories and for separable states indicates the steps involved.

The EPR paradox is not confined to position and momentum measurements on two sub-systems. A related paradox [93] occurs in the case of measurements on spin components $\widehat{S}_{\alpha 1}$ and $\widehat{S}_{\alpha 2}$—with $\alpha = x, y, z$—associated with two sub-systems 1 and 2. The spin operators also satisfy non-zero commutation rules (see paper II for details)

$$[\widehat{S}_{\alpha 1}, \widehat{S}_{\beta 1}] = {\rm i}\widehat{S}_{\gamma 1} \qquad [\widehat{S}_{\alpha 2}, \widehat{S}_{\beta 2}] = {\rm i}\widehat{S}_{\gamma 2}, \tag{38}$$

where α, β, γ are x, y, z in cyclic order. The question is whether the conditional variances $\langle \Delta \widehat{S}_{x1}^2 \rangle_{\widehat{S}_{x2}} \langle \Delta \widehat{x}_A^2 \rangle_{\widehat{x}_B}$ for measuring $\widehat{S}_{x1}$ for sub-system 1 having measured $\widehat{S}_{x2}$ for sub-system 2, and $\langle \Delta \widehat{S}_{y1}^2 \rangle_{\widehat{S}_{y2}}$ for measuring $\widehat{S}_{y1}$ for sub-system 1 having measured $\widehat{S}_{y2}$ for sub-system 2 violate the HUP

$$\langle \Delta \widehat{S}_{x1}^2 \rangle_{\widehat{S}_{x2}} \langle \Delta \widehat{S}_{y1}^2 \rangle_{\widehat{S}_{y2}} < \frac{1}{4} |\langle \widehat{S}_{z1} \rangle|^2. \tag{39}$$

Again we find that for separable states that the product of conditional variances $\langle \Delta \widehat{S}_{x1}^2 \rangle_{\widehat{S}_{x2}} \langle \Delta \widehat{S}_{y1}^2 \rangle_{\widehat{S}_{y2}} \geqslant \frac{1}{4} |\langle \widehat{S}_{z1} \rangle|^2$ showing that if the EPR violations as defined in (39) occur, then the state must be entangled. For completeness, this spin version of the EPR paradox is set out in appendix F.

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 $P_{AB}(\widehat{x}_A, x_A|\widehat{x}_B, x_B)$ or $P_{AB}(\widehat{p}_A, p_A|\widehat{x}_B, x_B)$. 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 $\widehat{x}_B$ are *recorded*, and not discarded. A discussion of EPR steering (see [19, 30]) is beyond the scope of this article.

2.6.2. Schrödinger cat paradox. The Schrödinger cat paradox [2, 94] relates to composite systems where one sub-system (the cat) is macroscopic and the other sub-system is microscopic (the radioactive atom). The paradox is a clear consequence of quantum theory allowing the existence of entangled states. Schrödinger 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 of one hour corresponding to the half-life for radioactive decay would be described in quantum theory via the entangled state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|e\rangle_{\rm Atom}|{\rm Alive}\rangle_{\rm Cat} + |g\rangle_{\rm Atom}|{\rm Dead}\rangle_{\rm Cat}) \tag{40}$$

in an obvious notation. The quantum state defined by (40) represents the knowledge that an observer outside the box would have about the combined atom-cat system one hour after the live cat was placed in the box along with an undecayed atom. The combined system is in an enclosed box, and opening the box and observing what is inside 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 was regarded as 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 Schrödinger 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. Thus the cat is *neither* dead *nor* alive until measurement has taken place when the box is opened. There is of course no paradox if the quantum state is only considered to represent the observer's information about what is inside the box. If the box is closed then at one half life after the cat was put into the box, the state vector (40) enables the outside observer to correctly assess the probability that the cat will be alive is $1/2$. If the box is then opened and the cat is found to be dead, then the observer's information changes and the state vector for the cat-atom system is now

$$|\Psi'\rangle = |g\rangle_{\rm Atom}|{\rm Dead}\rangle_{\rm Cat}\,. \tag{41}$$

In this interpretation of quantum states, the notion of there being some sort of underlying reality that exists *prior* to measurement is rejected. It is only this notion that such a reality must exist—perhaps described via hidden variables—that leads to the paradox. EPR paradoxes can also be constructed from the entangled state (40), as outlined in [95, 96].

In recent times, experiments based on a *Rydberg atom* in a *microwave cavity* [97] involving states such as (40) have been performed showing that entanglement can occur between macroscopic and microscopic systems, and it is even possible to prepare states analogous to $\frac{1}{\sqrt{2}}(|{\rm Alive}\rangle_{\rm Cat} + |{\rm Dead}\rangle_{\rm Cat})$ in the macroscopic system itself. In such experiments the different macroscopic states are large amplitude coherent states of the cavity mode. Coherent states are possible for *microwave photons* as they are created from *classical currents* with *well-defined phases*. A coherent superposition of an alive and dead cat within the cat sub-system itself can be *created* by measurement. The entangled state in (40) can also be written as

$$\begin{aligned}|\Psi\rangle = \frac{1}{\sqrt{2}}\Big\{&\frac{1}{\sqrt{2}}(|e\rangle_{\rm Atom} + |g\rangle_{\rm Atom})\frac{1}{\sqrt{2}}\\ &\times(|{\rm Alive}\rangle_{\rm Cat} + |{\rm Dead}\rangle_{\rm Cat})\\ &+\frac{1}{\sqrt{2}}(|e\rangle_{\rm Atom} - |g\rangle_{\rm Atom})\frac{1}{\sqrt{2}}\\ &\times(|{\rm Alive}\rangle_{\rm Cat} - |{\rm Dead}\rangle_{\rm Cat})\Big\}\end{aligned} \tag{42}$$

so that measurement on the atom for an observable in which the superposition states $\frac{1}{\sqrt{2}}(|e\rangle_{\rm Atom} \pm |g\rangle_{\rm Atom})$ are the eigen-states for this observable would result in the cat *then* being in the corresponding macroscopic superposition states $\frac{1}{\sqrt{2}}(|{\rm Alive}\rangle_{\rm Cat} \pm |{\rm Dead}\rangle_{\rm Cat})$ of an alive and dead cat.

2.7. Bell inequalities

Violations of Bell's Inequalities represent situations where neither HVT nor quantum theory based on separable states can account for the result, and therefore provide a clear case where an entangled quantum state is involved. Recent papers on Bell inequality violations include [8–11].

2.7.1. LHV result. A key feature of entangled states is that they are associated with *violations of Bell inequalities* [4] 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 Ω_A for sub-system A, which are listed A_1, A_2, etc, and two Ω_B for sub-system B, which are listed B_1, B_2, etc. The corresponding quantum Hermitian operators $\widehat{\Omega}_A$, $\widehat{\Omega}_B$, etc are $\widehat{A}_1$, $\widehat{A}_2$ and, $\widehat{B}_1$, $\widehat{B}_2$. The Bell inequalities involve the *mean value* $\langle A_i \times B_j\rangle_{\rm HVT}$ 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. For simplicity we consider a local HVT. In a LHV theory we see using (34) for Bell local states that the mean values $\langle A_i \times B_j\rangle_{\rm LHV}$ are given by

$$\langle A_i \times B_j\rangle_{\rm LHV} = \int {\rm d}\xi\, P(\xi)\langle A_i(\xi)\rangle\langle B_j(\xi)\rangle, \tag{43}$$

where $\langle A_i(\xi)\rangle$ and $\langle B_j(\xi)\rangle$ (as in equation (35)) are the values are assigned to A_i and B_j when the hidden variables are ξ, 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 between $+1$ and -1, since HVT does not conflict with quantum theory regarding allowed values for physical quantities. However, LHV 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* [86] for *Bell's inequality*is

$$|S| \leqslant 2, \tag{44}$$

where

$$\begin{aligned}S = &\langle A_1 \times B_1\rangle_{\rm LHV} + \langle A_1 \times B_2\rangle_{\rm LHV}\\ &+\langle A_2 \times B_1\rangle_{\rm LHV} - \langle A_2 \times B_2\rangle_{\rm LHV}\,.\end{aligned} \tag{45}$$

The minus sign can actually be attached to any one of the four terms The proof of this important result that all Bell local states must satisfy is given in [18] but for completeness is set out in appendix G.

2.7.2. Bell inequality violation and entanglement. We also confirm in appendix G that for a general two mode *non-entangled* state, $|S|$ cannot violate the Bell inequality upper bound of 2. This of course also follows directly from separable states being seen as examples of Bell local states. 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. An example of an entangled state that

violates the Bell inequality is the Bell state $|\Psi_-\rangle$ (see [18], section 2.5) written in terms of eigenstates of $\hat{\sigma}_z^A$ and $\hat{\sigma}_z^B$

$$|\Psi_-\rangle = \frac{1}{\sqrt{2}}(|+1\rangle_A \otimes |-1\rangle_B - |-1\rangle_A \otimes |+1\rangle_B) \quad (46)$$

we find that

$$E(\underset{\rightarrow}{a}\cdot\hat{\underset{\rightarrow}{\sigma}}^A \otimes \underset{\rightarrow}{b}\cdot\hat{\underset{\rightarrow}{\sigma}}^B) = -\underset{\rightarrow}{a}\cdot\underset{\rightarrow}{b}. \quad (47)$$

The Bell inequality given in the appendix equation (179) can be violated for the choice where $b_1$and b_2 are orthogonal and a_1, a_2 are parallel to $b_1 + b_2$, $b_1 - b_2$ respectively (see [18], section 5.1). Furthermore, such a quantum state cannot be described via a HVT, since Bell inequalities are always satisfied using a HVT. Experiments have been carried out in optical systems providing strong evidence for the existence of quantum states that violate Bell inequalities with only a few loopholes remaining (see [9, 19, 36] for references to experiments). Such violation of Bell inequalities is clearly a *non-classical* feature, since the experiments rule out all LHV theories. As Bell inequalities do not occur for separable states, the experimental observation of a Bell inequality indicates the presence of an entangled state. These violations are not without applications, since such Bell entangled states can be useful in device-independent quantum key distribution [17, 18, 36].

2.8. Non-local correlations

Another feature of entangled states is that they are associated with *strong correlations* for *observables* associated with *localized 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 HVT.

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

$$\langle\Omega_A^* \times \Omega_B\rangle_{\rm LHV} = \int \mathrm{d}\xi\, P(\xi)\Omega_A^*(\xi)\Omega_B(\xi)$$
$$\langle\Omega_A^*\Omega_A \times \Omega_B^*\Omega_B\rangle_{\rm LHV} = \int \mathrm{d}\xi\, P(\xi) \times \Omega_A^*(\xi)\Omega_A(\xi)\Omega_B^*(\xi)\Omega_B(\xi) \quad (48)$$

which then can be shown to satisfy the following *correlation inequality*

$$|\langle\Omega_A^* \times \Omega_B\rangle_{\rm LHV}|^2 \leqslant \langle\Omega_A^*\Omega_A \times \Omega_B^*\Omega_B\rangle_{\rm LHV}. \quad (49)$$

This result is based on the inequality

$$\int \mathrm{d}\xi\, P(\xi)C(\xi) \geqslant \left(\int \mathrm{d}\xi\, P(\xi)\sqrt{C(\xi)}\right)^2 \quad (50)$$

for real, positive functions $C(\xi)$, $P(\xi)$ and where $\int \mathrm{d}\xi\, P(\xi) = 1$, and which is proved in appendix E. 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 equation (49) is an indication of strong correlation between sub-systems A and B. It would also demonstrate Bell *non-locality*.

2.8.2. Correlation violation and entanglement. As separable states are particular cases of Bell local states it follows that the corresponding result to (49), namely

$$|\langle\widehat{\Omega}_A^\dagger \otimes \widehat{\Omega}_B\rangle|^2 = |\langle\widehat{\Omega}_A \otimes \widehat{\Omega}_B^\dagger\rangle|^2 \leqslant \langle\widehat{\Omega}_A^\dagger\widehat{\Omega}_A \otimes \widehat{\Omega}_B^\dagger\widehat{\Omega}_B\rangle \quad (51)$$

applies for separable states. The direct proof of this result is included for completeness in appendix H.

Hence if it is found that the correlation inequality is violated $|\langle\widehat{\Omega}_A^\dagger \otimes \widehat{\Omega}_B\rangle|^2 = |\langle\widehat{\Omega}_A \otimes \widehat{\Omega}_B^\dagger\rangle|^2 > \langle\widehat{\Omega}_A^\dagger\widehat{\Omega}_A \otimes \widehat{\Omega}_B^\dagger\widehat{\Omega}_B\rangle$ then the state must be entangled, so the correlation inequality violation is also a sufficiency test for *entanglement*.

3. Identical particles and entanglement

We now take into account the situation where systems of *identical particles* are involved. This requires us to give special consideration to the requirement that quantum states in such cases must conform to the *symmetrization principle* [58]. Further, entanglement is defined as a property that involves systems with two (or more) *sub-systems*, and the definition requires the specification of sub-systems that are *distinguishable* from each other and on which *measurements* can be made. In addition, the sub-systems must be able to exist as separate systems which can in principle be prepared in quantum states for that sub-system alone. This feature is vital to the definition of separable (or non-entangled) states on which the definition of entangled states is based. These key requirements that the sub-systems must be distinguishable, susceptible to measurements and can exist in separate quantum states are necessary for the concept of entanglement to make physical sense, and will have important consequences for the choice of sub-systems when identical particles are involved. These three key logical requirement for sub-systems rule out considering labeled identical particles as sub-systems and lead to the conclusion that sub-systems must be modes or sets of modes.

3.1. Symmetrization principle

Whether *entangled* or *not* the quantum states for systems of *identical particles* must conform to the *symmetrization principle*, whereby for mixed states the overall density operator has to be invariant under *permutation operators,* or if pure states are involved, the state vector is either unchanged (bosons) or changes sign (fermions) if the permutation operator is odd. Either a first quantization approach in which the basis states are written as *symmetrized products* of single particle states occupied by *labeled* identical particles can be used, or a second quantization approach where the basis states

are products of *Fock states* for all single particle states (modes), each Fock state specifying the *number* of identical particles occupying the particular mode. In first quantization the symmetrization process *removes* any distinction between identical particles, whereas in second quantization only *mode creation operators* are involved, and these do not involve labeled particles. Symmetrization is built into the definition of the Fock states. The two approaches are equivalent, but as we will see the second quantization approach is more suited to identifying sub-systems and defining entanglement in systems of identical particles.

3.1.1. General considerations. It is useful to clarify some of the issues involved by considering a simple example. Since density operators can always be expressed in a diagonal form involving their orthonormal eigenstates $|\Phi\rangle$ with real, positive eigenvalues $P(\Phi)$ as $\hat{\rho} = \sum_{\Phi} P(\Phi)|\Phi\rangle\langle\Phi|$ and each $|\Phi\rangle$ can always be written as a linear combination of basis vectors $|\Psi\rangle$, we will focus on these basis vectors and their forms in both first and second quantization. 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 α and β. In each case a particle has a choice of two modes which it may occupy. Thus there are two distinct single particle states (modes) designated as $|A\rangle$ and $|B\rangle$ in the *identical* particle case, and four distinct single particle states (modes) designated as $|A_\alpha\rangle$, $|B_\alpha\rangle$ and $|A_\beta\rangle$, $|B_\beta\rangle$ in the *distinguishable* particle case for particles α and β respectively. The notation in first quantization is that $|C(i)\rangle$ refers to a vector in which particle i is in mode $|C\rangle$. The notation in second quantization is that $|n\rangle_C$ refers to a vector where there are n particles in mode $|C\rangle$.

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

$$|\Psi\rangle_{\text{boson}} = \frac{1}{\sqrt{2}}(|A(1)\rangle \otimes |B(2)\rangle + |B(1)\rangle \otimes |A(2)\rangle), \tag{52}$$

$$|\Psi\rangle_{\text{fermion}} = \frac{1}{\sqrt{2}}(|A(1)\rangle \otimes |B(2)\rangle - |B(1)\rangle \otimes |A(2)\rangle) \tag{53}$$

and clearly satisfy the symmetrization principle. In *second quantization* the basis state in both the fermion and boson cases is

$$|\Psi\rangle_{\text{boson,fermion}} = |1\rangle_A \otimes |1\rangle_B. \tag{54}$$

In both first and second quantization this basis state involves one identical particle in mode $|A\rangle$ and the other in mode $|B\rangle$.

These examples highlight two possibilities for specifying *sub-systems* for systems of *identical* particles. The two possibilities have *differing* consequences in terms of whether specific pure states are regarded as separable or entangled in terms of the general form in equation (1) for separable pure states, depending on whether the first or second quantization approach is used. The *first option* is to regard the *labeled identical particles* as sub-systems—in which case using first quantization the boson or fermion basis states in equations (52) and (53) would be regarded as *entangled* states of the two sub-systems consisting of particle 1 and particle 2 [15, 74, 77]. This is a more mathematical approach, and suffers from the feature that the sub-systems are not distinguishable and measurements cannot be made on specifically labeled identical particles. In the case of identical particles the option of regarding labeled identical particles as the sub-systems leads to the concept of *entanglement due to symmetrization*. In the textbook by Peres ([15], see pp 126–8) it is stated that 'two particles of the same type are *always* entangled'. Peres obviously considers such entanglement is a result of symmetrization. The *second option* would be to regard the *modes* or single particle states as sub-systems [35] —in which case using second quantization the basis state for both fermions or bosons in equation (54) would be regarded as a *separable* state of two sub-systems consisting of modes $|A\rangle$ and $|B\rangle$. This is a more physically based approach, and has the advantage that the sub-systems are distinguishable and measurements can be made on specific modes. Noting that in the example the *same* quantum state is involved with one identical particle in mode $|A\rangle$ and the other in mode $|B\rangle$, the different categorization is disconcerting. It indicates that a choice must be made in regard to defining sub-systems when identical particles are involved (see section 3.1.2).

Now consider the case where the particles are *distinguishable*. Each distinguishable particle α, β has its own unique set of modes A_α, B_α, A_β, B_β. There are two cases in which one particle α occupies mode $|A_\alpha\rangle$ or $|B_\alpha\rangle$ and the other particle β occupies mode $|A_\beta\rangle$ or $|B_\beta\rangle$. Basis states analogous to the previous ones are given in *first quantization* as

$$\begin{aligned} |\Psi\rangle_{\text{dist}} &= |A_\alpha(\alpha)\rangle \otimes |B_\beta(\beta)\rangle \qquad \text{or} \\ |\Psi\rangle_{\text{dist}} &= |B_\alpha(\alpha)\rangle \otimes |A_\beta(\beta)\rangle. \end{aligned} \tag{55}$$

The somewhat surplus particle labels (α) and (β) have been added for comparison with (52) and (53). The states (57) are not required to satisfy the symmetrization principle since the particles are not identical. Each may be either a boson or a fermion. In *second quantization* the basis states are

$$\begin{aligned} |\Psi\rangle_{\text{dist}} &= (|1\rangle_{A_\alpha} \otimes |0\rangle_{B_\alpha}) \otimes (|0\rangle_{A_\beta} \otimes |1\rangle_{B_\beta}) \\ &\text{or} \\ |\Psi\rangle_{\text{dist}} &= (|0\rangle_{A_\alpha} \otimes |1\rangle_{B_\alpha}) \otimes (|1\rangle_{A_\beta} \otimes |0\rangle_{B_\beta}). \end{aligned} \tag{56}$$

In both first and second quantization, the first case corresponds to particle α being in mode $|A_\alpha\rangle$ and particle β being in mode $|B_\beta\rangle$ with the other two modes empty, and the second case corresponds to particle α being in mode $|B_\alpha\rangle$ and particle β being in mode $|A_\beta\rangle$ with the other two modes empty.

These examples also highlight two possibilities for specifying sub-systems for systems of *distinguishable* particles. In this case the two possibilities have *similar* consequences in terms of whether specific pure states are regarded as separable or entangled, based on the general form in equation (1) for separable pure states, irrespective of whether the first or second quantization approach is used. Here the *first option* is to regard the *labeled distinguishable*

particles as sub-systems—in which case using first quantization the boson or fermion basis states in equation (55) would be regarded as *separable* states of the two sub-systems consisting of particle α and particle β. The *second option* would be to regard the *modes* or single particle states as sub-systems—in which case using second quantization the basis state for both fermions or bosons in equation (56) would be regarded as a *separable* state of four sub-systems consisting of modes $|A_\alpha\rangle$, $|B_\alpha\rangle$ and $|A_\beta\rangle$, $|B_\beta\rangle$. Both expressions refer to the same quantum state, and the same result regarding separability is obtained in both first and second quantization, even though the number of sub-systems differ. It indicates that either option may be chosen in regard to defining sub-systems when distinguishable particles are involved. However, it is *simpler* if the same option—particles or modes as sub-systems—is made for treating either identical or distinguishable particle systems and we will adopt this approach.

To highlight the distinction between the identical and distinguishable particles situation, we note that for the two distinguishable particle case treated previously we can also form entangled states from the basis states (55) or (56)

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|A_\alpha(\alpha)\rangle \otimes |B_\beta(\beta)\rangle \pm |B_\alpha(\alpha)\rangle \otimes |A_\beta(\beta)\rangle) \tag{57}$$

which are similar in mathematical form to (52) and (53) when written in first quantization, and which are given by

$$|\Psi\rangle = \frac{1}{\sqrt{2}}((|1\rangle_{A_\alpha} \otimes |0\rangle_{B_\alpha}) \otimes (|0\rangle_{A_\beta} \otimes |1\rangle_{B_\beta}) \pm (|0\rangle_{A_\alpha} \otimes |1\rangle_{B_\alpha}) \otimes (|1\rangle_{A_\beta} \otimes |0\rangle_{B_\beta})) \tag{58}$$

when written in second quantization. However, in this case both the first and second quantization forms are clearly cases of *entangled* states. Whether they are regarded as entangled states of two sub-systems consisting of particle α and particle β (first option) or entangled states of the four sub-systems consisting of modes $|A_\alpha\rangle$, $|B_\alpha\rangle$ and $|A_\beta\rangle$, $|B_\beta\rangle$ (second option) depends on whether particle or modes are chosen as sub-systems.

Note however that *not* all basis states result in separable/entangled distinctions even in the case of identical particles. For the same two mode, two particle case as considered previously for bosons the basis vectors $|A(1)\rangle \otimes |A(2)\rangle$ or $|B(1)\rangle \otimes |B(2)\rangle$ (first quantization) or equivalently $|2\rangle_A \otimes |0\rangle_B$ or $|0\rangle_A \otimes |2\rangle_B$ (second quantization) would be regarded as separable states irrespective of whether particle or modes were chosen as the sub-systems. Entangled states such as $(|A(1)\rangle \otimes |A(2)\rangle \pm |B(1)\rangle \otimes |B(2)\rangle)/\sqrt{2}$ (first quantization) or equivalently $(|2\rangle_A \otimes |0\rangle_B \pm |0\rangle_A \otimes |2\rangle_B)/\sqrt{2}$ (second quantization) can also be formed from the two doubly occupied basis states. There are no analogous states for fermions due to the Pauli principle.

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 realize this may lead to states being regarded as separable when they are not (see section 3.4 for further examples).

In the above discussion the symmetrization principle was complied with both in the first and second quantization treatments. It should be noted however that some authors disregard the symmetrization principle. In describing BECs [74, 98] consider states of the form

$$\hat{\rho} = \sum_R P_R\, \hat{\rho}_R^1 \otimes \hat{\rho}_R^2 \otimes \hat{\rho}_R^3 \otimes \ldots \tag{59}$$

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

$$\hat{\rho} = P_{\sigma\xi}\, \hat{\sigma}^1 \otimes \hat{\xi}^2 + P_{\theta\eta}\, \hat{\theta}^1 \otimes \hat{\eta}^2 \tag{60}$$

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 $\hat{\rho} = P_\sigma\, \hat{\sigma}^1 \otimes \hat{\sigma}^2 + P_\theta\, \hat{\theta}^1 \otimes \hat{\theta}^2$. This is a statistical mixture of two states, one with *both* atoms in state $\hat{\sigma}$, the other with both atoms in state $\hat{\theta}$. Thus only special cases of (60) are compatible with the symmetrization principle. Of course if the atoms were all different (atom 1 a Rb^{87} atom, atom 2 a Na^{23} atom, ...) then the expression (60) would be a valid non-entangled state, but there the atomic sub-systems are distinguishable and symmetrization is not required. Such authors are really ignoring the symmetrization principle, and in addition are treating the individual identical particles in the BEC as separate sub-systems—a viewpoint we have described previously and will discuss further in the next section. For the present we just point out that valid quantum states must comply with the symmetrization principle.

3.1.2. Sub-systems—particles or modes? As highlighted in the previous section 3.1, when the quantum system involves identical particles the very definition of entanglement itself requires special care in regard to identifying legitimate sub-systems. There is a long-standing debate on the issue, with at present two schools of thought—see reviews such as [36] or [40]. As explained in the previous section, the *first* approach is to identify mathematically labeled individual identical *particles* as the sub-systems [15, 74, 77, 98]. Sub-systems may of course also be sets of such individually labeled particles. This approach leads to the conclusion that *symmetrization* creates entanglement of identical particles. The *second* approach is to identify single particle states or *modes* that the identical particles may occupy as the sub-systems [35]. The sub-systems may of course also be *sets* of distinguishable modes. This approach leads to the conclusion that it is *interaction processes* between modes that creates entanglement of distinguishable modes.

The approach based on *particle entanglement* is still being used [77]. As explained in section 3.1 this is not the same as mode entanglement so tests and measures for particle entanglement will differ from those for mode entanglement. A further discussion about the distinction is given in [41]. In a

recent paper Killoran *et al* [99] considered original states such as $(|a0(1)\rangle \otimes |a1(2)\rangle \pm |a0(2)\rangle \otimes |a1(1))/\sqrt{2}$ involving two modes $a0$ and $a1$—which were considered (based on first quantization) as an *entangled* state for two sub-systems consisting of particles 1 and 2, but would be considered (in second quantization) as a *separable* state $|1\rangle_{a0} \otimes |1\rangle_{a1}$ for two sub-systems consisting of modes $a0$ and $a1$. In addition there were two modes $b0$ and $b1$ which are initially unoccupied. The particles may be bosons or fermions. They envisaged converting such an input state using *interferometer* processes which couple A modes $a0$ and $a1$ to previously unoccupied B modes $b0$ and $b1$, into an output state—which is different. Projective measurements would then be made on the output state, based on having known numbers of particles in each of the A mode pairs $a0$ and $a1$ and in the B mode pairs $b0$ and $b1$. The projected state with one particle in the A modes and one particle in the B modes would be of the form (in second quantization) $(|1\rangle_{a0} \otimes |0\rangle_{a1} \otimes |0\rangle_{b0} \otimes |1\rangle_{b1} \pm |0\rangle_{a0} \otimes |1\rangle_{a1} \otimes |1\rangle_{b0} \otimes |0\rangle_{b1})/\sqrt{2}$, which is a bipartite entangled state for the two pairs of modes A and B and is *mathematically* of the same form as the first quantization *form* for the original A modes state considered as an example of *particle* entanglement if the correspondences $|a0(1)\rangle \rightarrow |1\rangle_{a0} \otimes |0\rangle_{a1}$, $|a1(2)\rangle \rightarrow |0\rangle_{b0} \otimes |1\rangle_{b1}$, $|a0(2)\rangle \rightarrow |1\rangle_{b0}|0\rangle_{b1}$ and $|a1(1)\rangle \rightarrow |0\rangle_{a0}|1\rangle_{a1}$ are made. Even the minus sign is obtained in the fermion case. Details are given in appendix I. Killoran *et al* stated that this represented a way of *extracting* the original symmetrization generated entanglement. However, another point of view is that the two mode interferometer process *created* an entangled state from a non-entangled state, and as the final measurements are still based on entanglement of modes it is hard to justify the claim that entanglement due to symmetrization exists as a directly observable basic feature in composite quantum systems—though the mapping identified in [99] is mathematically correct. Furthermore, all quantum states for identical particles are required to be symmetrized, so if symmetrization causes entanglement it differs from the numerous other controllable processes that produce entanglement by coupling the sub-systems. Since the idea of extracting entanglement due to symmetrization is of current interest, a fuller discussion of the approach by Killoran *et al* [99] is set out in appendix I.

However, it is generally recognized that sub-systems consisting of *individually labeled* identical particles are *not* amenable to *measurements*. What is distinguishable for systems of identical bosons or fermions 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 or fermionic atoms with several hyperfine components, each component will have its own set of modes. For photons the modes may be specified via wave vectors and polarizations. 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 suitable to use *second quantization*. Here, a basis set for the quantum states of such sub-systems are the *Fock states* $|n\rangle_A$ ($n = 0, 1, 2, \ldots$) 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 quantum states for this sub-system. Symmetrization is built into the definition of the Fock states, so the symmetrization principle is *automatically* adhered to. If the atoms were fermions rather than bosons the Pauli exclusion principle would of course restrict $n = 0, 1$ only. In this second quantization approach situations with differing *numbers* of identical particles are recognized as being different *states* of a system consisting of a set of modes, not different *systems* as would be the case in first quantization. The overall system will be associated with quantum states represented in the theory by 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. Finally, the artificial concept of entanglement due to symmetrization is replaced by the physically realistic concept of entanglement due to mode coupling.

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 [17, 33–35, 51, 52] and will be the approach used here—as in [5]. To emphasize—what are or are not entangled in the present treatment involving systems of identical particles are *distinguishable modes* not *labeled—indistinguishable—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.

As pointed out in section 3.1, in the case of systems consisting entirely of *distinguishable* particles the sub-systems may still be regarded as sets of modes, namely those single particle states associated with the particular distinguishable particle. In this case the particle descriptor (He atom, Na atom, ...) is synonymous with its collection of modes. Here all the sub-system states are one particle states.

3.1.3. Physical examples of modes. In terms of this approach, for non-interacting identical particles at zero temperature, the ground states for BECs and Fermi gases trapped in a harmonic potential provide examples of non-entangled states for bosonic and fermionic atoms respectively, when the sub-systems are chosen as the HO modes. In the bosonic case all the bosons occupy the lowest energy HO state, in the fermionic case one fermion occupies each HO state from the lowest up to a high energy state (the Fermi energy) until all the fermions are accommodated. On the other hand, if one particle position states spatially localized in two different regions are chosen as two sub-systems, then the same zero temperature state for the identical particle system is spatially entangled, as pointed out by Goold *et al* [39]. 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 $(|1\rangle_A|0\rangle_B + |0\rangle_A|1\rangle_B)/\sqrt{2}$ are entangled states. For entangled states associated with the EPR paradox or for quantum

teleportation, the mode functions may be *localized* in well-separated spatial regions—spooky action at a distance—but spatially overlapping mode functions apply in other situations. This distinction is important in discussions of quantum non-locality. Atoms in states with overall spin zero only have one internal state, but two mode systems can be created for their spatial motion using double-well trap potentials. If the wells are separated then two spatially separated modes can be created for studies of quantum non-locality. On the other hand atoms with spin $1/2$ have two internal states, which constitute a two mode system. However these two modes may be associated with the same or overlapping spatial wave functions, in which case studies of quantum non-locality are precluded. These latter situation can however still lead to what is referred to as intrasystem entanglement [100]. 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 and 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 equation (3) though the present paper mainly involves only two modes.

3.1.4. 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 section 4.3 of paper II, where *pairs* of modes associated with distinct lattice sites are considered as the sub-systems. Another example is treated in He *et al* [31], 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 sections 4.2 and 5.3 of paper II). A further example is treated by Heaney *et al* [101], 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.

3.2. Super-selection rule

As well as the symmetrization principle there is a further requirement that quantum states of systems of identical particles must satisfy—these are known as SSR*s*. These rules restrict the allowed quantum states of such systems to those in which the *coherences* between states with differing numbers of particles are zero. This applies at the global level for the overall quantum state, but also—as will be discussed in a later sub-section—to the sub-system states involved in the definition of separable or non-entangled states. The justification of the SSR at both the global and local level will be considered both in terms of simple physics arguments and in terms of reference frames. Examples of SSR and non-SSR compliant states will be given, both for overall states and for separable states. The validity of the SSR for the case of massive bosons or fermions is generally accepted, but in the case of photons there is doubt regarding their applicability. As papers I and II are focused on massive bosons, the situation for massless photons is discussed briefly in section 3.2.3 and then more fully in appendix L rather than in the main part of this paper. As pointed out in the Introduction, in the case of systems consisting entirely of single *distinguishable* particles the sub-systems may still be regarded as sets of modes, namely those single particle states associated with the particular distinguishable particle. Here all the sub-system states are one particle states and the overall system is an N particle state, so the local and global particle number SSRs, though true are irrelevant.

3.2.1. Global particle number SSR. The question of what quantum 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 SSR that prohibits *quantum superposition states* of the form

$$|\Phi\rangle = \sum_{N=0}^{\infty} C_N |N\rangle, \qquad \widehat{\rho} = \sum_{N=0}^{\infty} |C_N|^2 |N\rangle\langle N| + \sum_{N=0}^{\infty}\sum_{M=0}^{\infty} (1-\delta_{N,M}) C_N\, C_M^{*} |N\rangle\langle M| \tag{61}$$

being *quantum* 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 quantum states according to the SSR. The papers by Sanders *et al* [68] and Cable *et al* [102] 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 SSR indicates that the most *general quantum state* for a system of identical bosonic particles can only be of the form

$$\widehat{\rho} = \sum_{N=0}^{\infty}\sum_{\Phi} P_{\Phi N}\left(|\Phi_N\rangle\langle\Phi_N|\right), \qquad |\Phi_N\rangle = \sum_i C_i^N |N\ i\rangle, \tag{62}$$

where $|\Phi_N\rangle$ is a quantum superposition of states $|N\ i\rangle$ each of which involves exactly N particles, and where different states

with the same N are designated as $|N\ i\rangle$. This state $\widehat{\rho}$ 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

$$[\widehat{N},\ \widehat{\rho}] = 0, \tag{63}$$

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

3.2.2. Examples of global particle number ssr compliant states. Examples of a state vector $|\Phi_N\rangle$ for an entangled pure state [34] and a density operator $\widehat{\rho}$ for a non-entangled mixed [39] state for a *two mode bosonic* system, both of which are possible quantum states are

$$|\Phi_N\rangle = \sum_{k=0}^{N} C(N,\ k)|k\rangle_A \otimes |N-k\rangle_B, \tag{64}$$

$$\widehat{\rho} = \sum_{k=0}^{N} P(k)|k\rangle_A\langle k|_A \otimes |N-k\rangle_B\langle N-k|_B. \tag{65}$$

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

$$|\Phi_2\rangle = |1\rangle_A \otimes |1\rangle_B, \tag{66}$$

$$\widehat{\rho} = |1\rangle_A\langle 1|_A \otimes |1\rangle_B\langle 1|_B. \tag{67}$$

Neither state is entangled and both are the same pure state since $\widehat{\rho} = |\Phi_2\rangle\langle\Phi_2|$. Although the SSRs and symmetrization 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.

Bell states [17, 18] for $N = 1$ bosons provide important examples of entangled two mode pure quantum states that are compliant with the global particle number SSR. The modes are designated A, B and the Fock states are in general $|n_A,\ n_B\rangle$. These Bell states may be written

$$|\Psi_{AB}^{-}\rangle = \frac{1}{\sqrt{2}}(|0_A,\ 1_B\rangle - |1_A,\ 0_B\rangle)$$
$$|\Psi_{AB}^{+}\rangle = \frac{1}{\sqrt{2}}(|0_A,\ 1_B\rangle + |1_A,\ 0_B\rangle) \tag{68}$$

Neither of these states is separable. There are also two other two mode Bell states given by

$$|\Phi_{AB}^{-}\rangle = \frac{1}{\sqrt{2}}(|0_A,\ 0_B\rangle - |1_A,\ 1_B\rangle)$$
$$|\Phi_{AB}^{+}\rangle = \frac{1}{\sqrt{2}}(|0_A,\ 0_B\rangle + |1_A,\ 1_B\rangle). \tag{69}$$

These however are not compliant with the global particle number SSR. Linear combinations $(|\Phi_{AB}^{-}\rangle + |\Phi_{AB}^{+}\rangle)/\sqrt{2} = |0_A,\ 0_B\rangle$ and $(-|\Phi_{AB}^{-}\rangle + |\Phi_{AB}^{+}\rangle)/\sqrt{2} = |1_A,\ 1_B\rangle$ are global particle number SSR compliant and also separable, corresponding to states with $N = 0$ and $N = 2$ bosons respectively.

3.2.3. SSRs and conservation laws. It is important to realize that such SSRs [59] are *different constraints* to those imposed by *conservation laws*, as emphasized by Bartlett *et al* [67]. 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. They are however related, as is discussed in section 3.3.1 and appendix K where the SSRs based on particle number are related to invariances of the density operator under changes of phase reference frames. This involves considering groups of phase changing operators $\widehat{T}(\theta_a) = \exp(\mathrm{i}\widehat{N}_a\theta_a)$ when considering local particle number SSR for single modes in the context of separable states, or $\widehat{T}(\theta) = \exp(\mathrm{i}\widehat{N}\theta)$ when considering global particle number SSR in the context of multimode entangled states. SSRs 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 SSRs on both charge and baryon number preclude such states. The basis quantum states for such a combined system would involve symmetrized tensor products of hydrogen atom and helium ion states, not linear combinations—symmetrization being required because the system contains two identical electrons. On the other hand, SSRs 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 quantum states.

However, conservation laws on total particle number (such as apply in the case of massive bosons) are relevant to showing that multi-mode states generated via total particle number conserving processes from an initial separable state will be global SSR compliant if the sub-systems in the initial state are local particle number SSR compliant, and will not be if the initial state involves a sub-system state that is not local particle number SSR compliant. For simplicity we consider two sub-systems A and B with the initial state

$$\widehat{\rho}(0) = \sum_R P_R\ \widehat{\rho}_R^A \otimes \widehat{\rho}_R^B. \tag{70}$$

If $\widehat{U}(t)$ is the evolution operator where $\widehat{\rho}(t) = \widehat{U}(t)\widehat{\rho}(0)\widehat{U}(t)^{\dagger}$ and the processes are number conserving

then $[\widehat{N},\,\widehat{U}\,(t)]=0$. We then have

$$[\widehat{N},\,\widehat{\rho}\,(t)]=\widehat{U}\,(t)[\widehat{N},\,\widehat{\rho}\,(0)]\,\widehat{U}\,(t)^{\dagger}$$
$$=\widehat{U}\,(t)\sum_{R}P_{R}([\widehat{N}_{A},\,\widehat{\rho}_{R}^{A}]\otimes\widehat{\rho}_{R}^{B}$$
$$+\,\widehat{\rho}_{R}^{A}\otimes[\widehat{N}_{B},\,\widehat{\rho}_{R}^{B}])\,\widehat{U}\,(t)^{\dagger}. \tag{71}$$

Hence if $\widehat{\rho}_{R}^{A}$ and $\widehat{\rho}_{R}^{B}$ are local particle number SSR compliant, then $[\widehat{N}_{A},\,\widehat{\rho}_{R}^{A}]$ and $[\widehat{N}_{B},\,\widehat{\rho}_{R}^{B}]$ are zero, showing that $[\widehat{N},\,\widehat{\rho}\,(t)]=0$ so the state is global particle number SSR compliant. On the other hand if $[\widehat{N},\,\widehat{\rho}\,(t)]=0$ we see that $[\widehat{N},\,\widehat{\rho}\,(0)]=\sum_{R}P_{R}([\widehat{N}_{A},\,\widehat{\rho}_{R}^{A}]\otimes\widehat{\rho}_{R}^{B}+\widehat{\rho}_{R}^{A}\otimes[\widehat{N}_{B},\,\widehat{\rho}_{R}^{B}])=0$. By taking Tr_{A} and Tr_{B} of this result gives $\sum_{R}P_{R}[\widehat{N}_{A},\,\widehat{\rho}_{R}^{A}]=\sum_{R}P_{R}\,[\widehat{N}_{B},\,\widehat{\rho}_{R}^{B}]=0$. This shows that both of the reduced density operators $\sum_{R}P_{R}\widehat{\rho}_{R}^{A}$ and $\sum_{R}P_{R}\widehat{\rho}_{R}^{B}$ must be local particle number SSR compliant, which amounts to requiring the sub-system density operators to be local particle number SSR compliant. This situation applies even when there is coupling between modes, provided the interaction is number conserving—such as a coupling given by $\widehat{V}=\lambda\hat{a}\hat{b}^{\dagger}+HC$. Analogous results apply for systems of massive bosons if there are more than two modes involved, where again global SSR compliance involves the total particle number since even with interactions there is total number conservation. For example with three modes in coupled BECs, interactions of the form $\widehat{V}=\lambda(\hat{c})^{2}\hat{a}^{\dagger}\hat{b}^{\dagger}+HC$ in which two bosons are annihilated in mode C and one boson is created in each of modes A and B are consistent with total particle number conservation and lead to global SSR involving the total particle number.

Although outside the focus of this paper, it is worth pointing out that somewhat different considerations apply to *photons*. Single non-interacting modes, such as are discussed in the context of separable states do have a conservation law for the photon number in that mode. The applicability (or otherwise) of the local particle number SSR for the sub-system density operators in a separable state is discussed in appendix L. In the case of interacting photonic modes there may be no conservation law associated with total photon number and it may be thought that no global SSR would apply. However, other global SSR involving combinations of the mode photon numbers may still apply. As an example, we consider a three mode situation in a non-degenerate parametric amplifier, where the basic generation process involves one pump photon of frequency $\omega_{C}=\omega_{A}+\omega_{B}$ being destroyed and one photon created in each of modes A and B. The interaction term is $\widehat{V}=\lambda\hat{c}\hat{a}^{\dagger}\hat{b}^{\dagger}+HC$. It is straightforward to show that a total *quanta* number operator $\widehat{N}_{\mathrm{tot}}=\widehat{N}_{A}+\widehat{N}_{B}+2\widehat{N}_{C}$ commutes with the Hamiltonian. The situation is analogous to the atom–molecule system treated in appendix M. Thus $\widehat{N}_{\mathrm{tot}}$ is conserved and we can then consider a group of phase changing operators $\widehat{T}\,(\theta)=\exp(\mathrm{i}\widehat{N}_{\mathrm{tot}}\theta)$ and show that there could be a global SSR for the three mode system, but now involving the total quanta number $N_{A}+N_{B}+2N_{C}$. The pure state which is often used in a quantum treatment of the non-degenerate parametric amplifier $|\Psi\rangle=\sum_{n}C_{n}\,|n\rangle_{A}\otimes|n\rangle_{B}\otimes|N-n\rangle_{C}$ is global SSR compliant in terms of the modified $\widehat{N}_{\mathrm{tot}}$, since in every term $N_{A}+N_{B}+2N_{C}=2N$ and there are no coherences between terms with different N_{tot}. For the non-degenerate parametric amplifier case an analogous treatment to that for number conserving processes shows that if

$$\widehat{\rho}\,(0)=\sum_{R}P_{R}\,\widehat{\rho}_{R}^{A}\otimes\widehat{\rho}_{R}^{B}\otimes\widehat{\rho}_{R}^{C} \tag{72}$$

then using $[\widehat{N}_{\mathrm{tot}},\,\widehat{U}\,(t)]=0$ we have

$$[\widehat{N}_{\mathrm{tot}},\,\widehat{\rho}\,(t)]=\widehat{U}\,(t)[\widehat{N}_{\mathrm{tot}},\,\widehat{\rho}\,(0)]\,\widehat{U}\,(t)^{\dagger}=\widehat{U}\,(t)\sum_{R}P_{R}$$
$$\times\begin{pmatrix}[\widehat{N}_{A},\,\widehat{\rho}_{R}^{A}]\otimes\widehat{\rho}_{R}^{B}\otimes\widehat{\rho}_{R}^{C}+\widehat{\rho}_{R}^{A}\otimes[\widehat{N}_{B},\,\widehat{\rho}_{R}^{B}]\otimes\widehat{\rho}_{R}^{C}\\+2\widehat{\rho}_{R}^{A}\otimes\widehat{\rho}_{R}^{B}\otimes[\widehat{N}_{C},\,\widehat{\rho}_{R}^{C}]\end{pmatrix}\widehat{U}\,(t)^{\dagger}. \tag{73}$$

Hence if $\widehat{\rho}_{R}^{A}$, $\widehat{\rho}_{R}^{B}$ and $\widehat{\rho}_{R}^{C}$ are local particle number SSR compliant, then $[\widehat{N}_{\mathrm{tot}},\,\widehat{\rho}\,(t)]=0$ so the state is SSR compliant, but with global total quanta number $\widehat{N}_{\mathrm{tot}}$. On the other hand if $[\widehat{N}_{\mathrm{tot}},\,\widehat{\rho}\,(t)]=0$ we find that $\sum_{R}P_{R}\,[\widehat{N}_{A},\,\widehat{\rho}_{R}^{A}]=\sum_{R}P_{R}\,[\widehat{N}_{B},\,\widehat{\rho}_{R}^{B}]=\sum_{R}P_{R}\,[\widehat{N}_{C},\,\widehat{\rho}_{R}^{C}]=0$. This shows that each of the reduced density operators $\sum_{R}P_{R}\widehat{\rho}_{R}^{A}$, $\sum_{R}P_{R}\widehat{\rho}_{R}^{B}$ and $\sum_{R}P_{R}\widehat{\rho}_{R}^{C}$ must be local particle number SSR compliant, which amounts to requiring the sub-system density operators to be local particle number SSR compliant.

3.2.4. SSR justification and no suitable phase reference. There are two types of justification for applying the SSRs for systems of identical particles. The first approach is based on simple considerations and will be outlined below in this subsection. The second approach [40, 60, 63, 64, 66–71] 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 K. 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, while 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 $\widehat{\rho}$ used to describe the various quantum states will be that of the external observer (Charlie).

There is a further reference frame based justification for the SSRs proposed by Stenholm [103] involving Galilean transformations—corresponding to describing the system from the point of view of an observer moving with a constant velocity with respect to the original observer, and where the two observers have identical clocks. A consideration of where the relative velocity is unknown might lead to the conclusion that SSR non-compliant coherences do not occur. For completeness, a brief discussion is included in appendix K.

3.2.5. 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 (61) as quantum 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

$$|\Phi\rangle = \sum_{m=0}^{M} C_m \, |M-m\rangle_{\rm mol} \otimes |2m\rangle_{\rm atom} \tag{74}$$

but the reduced density operator for the bosonic atoms is

$$\widehat{\rho}_{\rm atoms} = \sum_{m=0}^{M} |C_m|^2 \, (|2m\rangle \, \langle 2m|)_{\rm atom} \tag{75}$$

which is a statistical mixture of states with differing atom numbers with no coherence terms between such states. Such statistical mixtures are valid quantum 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

$$|\Phi\rangle = \sum_{m=0}^{M} B_m \, |M-m\rangle_{\rm mol} \otimes \sum_{n=0}^{M} A_{2n} \, |2n\rangle_{\rm atom}, \tag{76}$$

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 product of coefficient $B_m A_{2n}$ involving product states $|M-m\rangle_{\rm mol} \otimes |2n\rangle_{\rm atom}$ with $n \neq m$ if the state $|\Phi\rangle$ is not just in the entangled form (74). 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 (61) did exist then the amplitudes C_N would oscillate with frequencies that differ by frequencies of order $\omega_C = mc^2/\hbar$ (the Compton frequency, which is $\gtrsim 10^{25}$ Hz for massive bosons) even if boson–boson interactions were included Suppose a SSR violating state such as (61) could be created. To distinguish the phases of the C_N in order to verify the existence of the non-SSR-complying state, we need to measure the *mean value* $\langle \widehat{\Omega}_A \rangle$ of observables—such as *quadrature* operators in the case of a single mode $\widehat{x}_A = (\widehat{a} + \widehat{a}^\dagger)/\sqrt{2}$ and $\widehat{p}_A = (\widehat{a} - \widehat{a}^\dagger)/\mathrm{i}\sqrt{2}$,—which have non-zero matrix elements between states with differing N. To observe the oscillations in $\langle \widehat{\Omega}_A \rangle$ that would demonstrate the existence of a non-SSR-complying state, the mean value $\langle \widehat{\Omega}_A \rangle$ of such an observable would need to change by a *detectable* amount in a time scale Δt short compared to the period of the oscillations—that is, short compared to the Compton period $2\pi/\omega_C$. A reasonable measure for the minimal detectable change would be the original standard deviation $\Delta\Omega_A = \sqrt{\langle \Delta\widehat{\Omega}_A^2 \rangle}$ for measurements on $\widehat{\Omega}_A$ (where the fluctuation is $\Delta\widehat{\Omega}_A = \widehat{\Omega}_A - \langle \widehat{\Omega}_A \rangle$). However there is an *uncertainty principle* relationship between the time scale Δt during which the mean value changes by a standard deviation and the standard deviation in the *energy* $\Delta H_A = \sqrt{\langle \Delta\widehat{H}_A^2 \rangle}$ that applies for the quantum state being studied, namely $\Delta H_A \, \Delta t \geqslant \hbar/2$. As we have seen, we require $\Delta t \ll 2\pi/\omega_C$ so that from the energy–time uncertainty principle we see that $\Delta H_A \gg \hbar\omega_C = mc^2$. The consequence is that the uncertainty in energy for the proposed SSR violating quantum state must be large compared to the *rest mass energy* in order to observe the effects of SSR-non-compliance. This shows that the proposed observation is not possible for the *non-relativistic* quantum systems we are considering, since the energy uncertainty is large enough to allow the existence of boson–anti-boson pairs. This argument about the non-observability of non-SSR-complying states in the case of massive particles is an in-principle demonstration that the SSR non-complying oscillations are too large to be followed, and is much stronger than one that is merely based on the current lack of an appropriate technology. We note in passing that the same discussion does *not* apply to *photons*, whose rest mass energy is zero.

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 [78] has pointed out (see also Bach *et al* [104], Dalton and Ghanbari [38]), 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 [68, 102, 105].

3.2.6. Global SSR compliant states and quantum correlation functions. We now prove a theorem concerning *quantum correlation functions* for bosonic systems with two modes A

and B. This theorem is relevant for possible tests on whether the SSR apply, as we will see in the next section.

Theorem. *If a state is global particle number SSR compliant then all quantum correlation functions* $\langle(\hat{a}^\dagger)^n(\hat{a})^m(\hat{b}^\dagger)^l(\hat{b})^k\rangle$ *for which* $n+l\neq m+k$ *must be zero. The proof of this theorem is given in appendix J.*

3.2.7. Testing the SSRs. The last result for the general two mode quantum correlation function $\langle(\hat{a}^\dagger)^n(\hat{a})^m(\hat{b}^\dagger)^l(\hat{b})^k\rangle$ is relevant to the various experimental measurements that are discussed in the accompanying paper II. For example, as we will see $\langle\hat{S}_x\rangle_\rho$ is a combination of $\langle(\hat{a}^\dagger)^n(\hat{a})^m(\hat{b}^\dagger)^l(\hat{b})^k\rangle$ with $n=1, m=0, l=0, k=1$ and $n=0, m=1, l=1, k=0$, and $\langle\Delta\hat{S}_x^2\rangle_\rho=\langle\hat{S}_x^2\rangle_\rho-\langle\hat{S}_x\rangle_\rho^2$ would involve terms such as $\langle(\hat{a}^\dagger)^n(\hat{a})^m(\hat{b}^\dagger)^l(\hat{b})^k\rangle$ with $n=2, m=0, l=0, k=2$ and $n=0, m=2, l=2, k=0$, and $n=1, m=1, l=1, k=1$ from $\langle\hat{S}_x^2\rangle_\rho$. All of these have $n+l=m+k$, so they can be non-zero for globally SSR compliant states. The question then arises—what sort of quantity of the form $\langle(\hat{a}^\dagger)^n(\hat{a})^m(\hat{b}^\dagger)^l(\hat{b})^k\rangle$ could be used to see if the quantum state was not globally SSR compliant? The answer is seen in terms of two corollaries to the last theorem. The proof of these corollaries is given in appendix J.

Corollary 1. *If we find that any of the quantum correlation functions* $\langle(\hat{a}^\dagger)^n(\hat{a})^m(\hat{b}^\dagger)^l(\hat{b})^k\rangle$ *are non-zero when* $n+l\neq m+k$ *then the state is not global particle number SSR compliant.*

Corollary 2. *Measurements of the QCF* $\langle(\hat{a}^\dagger)^n(\hat{a})^m(\hat{b}^\dagger)^l(\hat{b})^k\rangle$ *when* $n+l=m+k$ *cannot determine whether or not the state includes a contribution that is global particle number SSR non-compliant.*

The first corollary indicates what type of measurement is needed to see if SSR non compliant states exist. Quantities of the type $\langle(\hat{a}^\dagger)^n(\hat{a})^m(\hat{b}^\dagger)^l(\hat{b})^k\rangle$ are measured for which $n+l\neq m+k$. If we find *any* that are non-zero we can then conclude that we have found a state which is *not* global particle number SSR compliant. The second corollary shows that measurements of this type with $n+l=m+k$ would *not* respond to the presence of contribution to the density operator that is not globally SSR compliant.

Hence the *conclusion* is that a quantum correlation function of the form $\langle(\hat{a}^\dagger)^n(\hat{a})^m(\hat{b}^\dagger)^l(\hat{b})^k\rangle$ must be measured for cases where $n+l\neq m+k$ *and* a non-zero measurement result must be found. If it is, then we would have demonstrated that the state is not globally SSR compliant. The simplest case would be to find a non-zero result for $\langle\hat{a}\rangle_\rho$ or $\langle\hat{b}\rangle_\rho$.

Similar considerations apply to *local* SSR *compliance* in the sub-system states. For sub-system a a QCF of the form $\langle(\hat{a}^\dagger)^n(\hat{a})^m\rangle$ must be measured for cases where $n\neq m$ and a non-zero measurement result must be found. If it is, then we would have demonstrated that the state is not locally SSR compliant. The simplest case would be to find a non-zero result for $\langle\hat{a}\rangle_\rho$.

3.2.8. Particle entanglement measure. Various measures of entanglement have been referred to in the Introduction. The so-called *particle entanglement measure* is one that takes into account both the SSR and particle identity. Wiseman *et al* have also treated entanglement for pure states [45] and mixed states [106] in identical particle systems, applying both the symmetrization principle and SSRs, invoking the argument that *without* a phase reference the quantum state must be comply with the local (and global) particle number SSR. This is essentially the same approach as in [5, 60, 71] and in the present paper. For two mode systems the *observable* system density operator $\tilde{\hat{\rho}}$ is obtained from the density operator $\hat{\rho}$ that would apply *if* such a phase reference existed via the expression

$$\tilde{\hat{\rho}}=\sum_{n_An_B}\hat{\Pi}_{n_An_B}\,\hat{\rho}\,\hat{\Pi}_{n_An_B}=\sum_{n_An_B}\hat{\rho}^{(n_An_B)}, \tag{77}$$

where $\hat{\Pi}_{n_An_B}=\hat{\Pi}^2_{n_An_B}$ is a projector onto sub-system states with n_A, n_B particles in modes A, B respectively. Note that $\hat{\rho}^{(n_An_B)}=\hat{\Pi}_{n_An_B}\,\hat{\rho}\,\hat{\Pi}_{n_An_B}$ is not normalized to unity. In fact the probability that there are n_A, n_B particles in modes A, B respectively is given by $P_{n_An_B}=\mathrm{Tr}(\hat{\Pi}_{n_An_B}\,\hat{\rho}\,\hat{\Pi}_{n_An_B})=\mathrm{Tr}(\hat{\rho}^{(n_An_B)})$, so $\mathrm{Tr}(\tilde{\hat{\rho}})=\sum_{n_An_B}P_{n_An_B}=1$. For *separable* states defined here as in equation (3), the expression in (77) for the density operator is the *same* as that used here, since with $\hat{\rho}$ given by equation (3) and with $\sum_{n_An_B}\hat{\Pi}_{n_An_B}(\hat{\rho}_R^A\otimes\hat{\rho}_R^B)\hat{\Pi}_{n_An_B}=\hat{\rho}_R^A\otimes\hat{\rho}_R^B$ it is easy to show that $\tilde{\hat{\rho}}=\hat{\rho}_{\mathrm{sep}}$. For general mixed states Wiseman *et al* introduce in [45] the idea of *particle entanglement* by defining its measure $E_P(\hat{\rho}\,)$ by

$$E_P(\hat{\rho}\,)=\sum_{n_An_B}P_{n_An_B}E_M(\hat{\rho}^{(n_An_B)})=E_P(\tilde{\hat{\rho}}\,), \tag{78}$$

where $E_M(\hat{\rho}^{(n_An_B)})$ is a measure of the *mode entanglement* associated with the (unnormalized) state $\hat{\rho}^{(n_An_B)}$. This might be taken as the *entropy* of mode entanglement $E_M(\hat{\sigma})=-\mathrm{Tr}(\hat{\sigma}_A\ln\hat{\sigma}_A)$ for normalized density operators $\hat{\sigma}$, where the reduced density operator for mode A is $\hat{\sigma}_A=\mathrm{Tr}_B(\hat{\sigma})$. Note that from $\hat{\Pi}_{n_An_B}\hat{\Pi}_{m_Am_B}=\delta_{n_Am_A}\delta_{n_Bm_B}\hat{\Pi}_{n_An_B}$ the particle entanglement measure $E_P(\hat{\rho})$ is the same for $\tilde{\hat{\rho}}$, the observable density operator for the system. The *operational definition* of E_P is the maximal amount of entanglement which can be produced between the two (non-SSR-constrained sub-systems by local operations. In the case of the separable state for modes A, B given in (3) it is straightforward to show that

$$\hat{\rho}_{\mathrm{sep}}^{(n_An_B)}=\sum_R P_R(\hat{\Pi}_{n_A}\hat{\rho}_R^A\,\hat{\Pi}_{n_A})\otimes(\hat{\Pi}_{n_B}\hat{\rho}_R^B\,\hat{\Pi}_{n_B}), \tag{79}$$

$$P_{n_An_B}^{\mathrm{sep}}=\sum_R P_R\,P_{n_A}(\hat{\rho}_R^A)P_{n_B}(\hat{\rho}_R^B), \tag{80}$$

where $\hat{\Pi}_{n_A}$ and $\hat{\Pi}_{n_B}$ are projectors onto sub-system states in modes A, B respectively with n_A and n_B particles in the respective modes $(\hat{\Pi}_{n_An_B}=\hat{\Pi}_{n_A}\otimes\hat{\Pi}_{n_B})$, with $P_{n_A}(\hat{\rho}_R^A)=\mathrm{Tr}_A(\hat{\Pi}_{n_A}\hat{\rho}_R^A)$ and $P_{n_B}(\hat{\rho}_R^B)=\mathrm{Tr}_B(\hat{\Pi}_{n_B}\hat{\rho}_R^B)$ being the probabilities of finding n_A and n_B particles in the

respective modes when the corresponding sub-system states are $\widehat{\rho}_R^A$ and $\widehat{\rho}_R^B$. Since the state $\widehat{\rho}_{\rm sep}^{(n_A n_B)}$ is clearly a separable state of the form (3) for the modes A, B, the corresponding measure of mode entanglement must be zero. It then follows from the general expression (78) that the particle entanglement measure is also zero for the separable state. This is as expected.

$$E_P(\widehat{\rho}_{\rm sep}) = 0. \tag{81}$$

For the pure states considered in [45] we note that among them is the two boson state $|1\rangle_A \otimes |1\rangle_B$ which has one boson in each of the two modes A, B. The particle entanglement measure $E_P(\widehat{\rho})$ is zero for this state (where $\widehat{\rho} = (|1\rangle\langle 1)_A \otimes (|1\rangle\langle 1)_B$), consistent with it being a separable rather than an entangled state. This indicates that Wiseman *et al* [45] do *not* consider that entanglement occurs due to symmetrization, as the first quantization form for the state might indicate. However, finding $E_P(\widehat{\rho})$ to be zero does not always shows that the state is separable, as the case of the *relative phase state* (defined in appendix O of paper II, see also [38]) shows. As is shown there, $E_P(\widehat{\rho}) = 0$ for the relative phase state, yet the state is clearly an entangled one. Just as some entangled states have zero spin squeezing, some entangled states may be associated with a zero particle entanglement measure. Nevertheless a non-zero result for the particle entanglement measure $E_P(\widehat{\rho})$ *shows* that the state must be *entangled*—again we have a *sufficiency* test. However, as in the case of other entanglement measures the problem with using the particle entanglement measure to detect entangled states is that there is no obvious way to measure it experimentally.

3.3. Reference frames and violations of superselection rules

Challenges to the requirement for quantum states to be consistent with SSRs have occurred since the 1960s when Aharonov and Susskind [66] suggested that coherent superpositions of different charge eigenstates could be created. It is argued that SSRs 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—[40, 60, 63, 64, 66–71] provide discussions regarding reference systems and SSR.

3.3.1. Linking SSR and reference frames. The discussion of the SSR 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 K. The key idea is that there are two observers—Alice and Charlie—who are describing the same prepared system in terms of their own reference frames and hence their descriptions involve two different quantum states. The reference systems are *macroscopic systems* in states where the behavior 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 $\widehat{T}(g)$, 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 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 appendix equation (221) for Situation A and appendix equation (222) 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 behavior 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 appendix equation (246)). 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 appendix equations (251) and (252)). 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.

3.3.2. Can coherent superpositions of atom and molecules occur? Based around the reference frame approach Dowling *et al* [106] and Terra Cunha *et al* [35] 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 [106]. Dunningham *et al* [107] consider a scheme for observing a superposition of a one boson state and the vacuum state. Obviously if SSRs 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 $\overline{N} \sim 10^8$ 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 SSRs rather than coherent superpositions, which are only present in Alice's description of the state (see appendix K). Also, although coherence and interference effects are demonstrated, these can also be accounted for without invoking the presence of coherent superpositions that violate the SSRe. As the paper by Dowling *et al* [106] entitled 'Observing a coherent superposition of an atom and a molecule' is a good example of where the SSRs are challenged, the key points are described in appendix M. 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 Δ for a time τ 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 M 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 ϕ 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 ϕ imparted during the process that demonstrates coherence (Ramsey interferometry) effects, but it is shown in appendix M 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 SSR has not been demonstrated via this particular process.

3.3.3. Detection of SSR violating states. Whether such SSR 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 [107]). 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 τ 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 ϕ. Details are given in appendix M. There is no dependence on the relative phase between α and β, 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 $\hat{\rho}(i) = |\alpha|^2 (|0\rangle_A \langle 0|_A \otimes |0\rangle_B \langle 0|_B) + |\beta|^2 (|1\rangle_A \langle 1|_A \otimes |0\rangle_B \langle 0|_B)$, 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 proposed coherent superposition associated with the SSR violating state would not be detected in this interferometric process, nor in the more elaborate scheme discussed in [107].

Of course, the claim that in isolated systems of *massive* particles it is not possible in *non-relativistic quantum physics* to create states that violate the particle number SSR—either for the sub-system states in a separable state or for any quantum state of the overall system—can be questioned. Ideally the claim should be *tested* by experiment, in particular when the number of particles is large in view of the interest in *macroscopic entanglement* since the Schrödinger cat was first described. The simplest situation would be to test whether states that violate the (local) particle number SSR could be created for a *single mode system*. Clearly, a specific *proposal* for an experiment in which the SSR *could* be violated is required, but to our knowledge no such proposal has been presented. BECs, in which all the bosons can occupy a single mode would seem an ideal candidate as a suitable bosonic system, and the *Glauber coherent state* is an example of a non-SSR compliant state. For fermions, the Pauli exclusion principle would limit the number of fermions in a one mode system to be zero or one, but coherent superpositions of a zero and one fermion state are examples of non-SSR compliant pure states. As pointed out above, some authors such as [56, 57, 61, 62], base their definition of entanglement by allowing for the possible presence of non-SSR compliant sub-system states when defining separable states. The approach in [5] is based on the *physical assumption* that states that are non-compliant with particle number SSR—both local and global—do *not* come into the realm of non-relativistic

quantum physics, in which the concept of entanglement is useful. Until *clear evidence* is presented that non-SSR-compliant states *can* be prepared, and in view of the theoretical reasons why they *cannot*, it seems preferable to base the *theory of entanglement* on their *absence* when defining separable and entangled quantum states.

3.4. SSR—separate sub-systems

In this sub-section the important case of SSR in *separable* states will be dealt with, since this is key to understanding what entangled states are allowed in systems involving identical particles. This forms the basis for the treatment of entanglement tests presented in the second part of this review (paper II).

3.4.1. Local particle number SSR. We now consider the role of the SSR for the case of *non-entangled* states. The global SSR on *total particle number* has restricted the physical quantum state for a system of identical bosons to be of the form (62). 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 $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, ... 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

$$[\widehat{N}_X, \widehat{\rho}_R^X] = 0, \tag{82}$$

where $\widehat{N}_X$ is the *number* operator for sub-system $X = A, B, \ldots$ .The SSR restriction is based on the proposition that the density operators $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, ... for the separate sub-systems A, B, ... should themselves represent possible *quantum states* for each of the sub-systems, considered as a *separate system* and thus be required to satisfy the SSR that forbids quantum superpositions of Fock states with differing boson numbers. Note that if the local particle number SSR applies in each sub-system the global particle number SSR applies to any separable state. The proof is trivial and just requires showing that $[\widehat{N}, \widehat{\rho}_{\rm sep}] = 0$

The justification of applying the *local particle number* SSR to the density operators $\widehat{\rho}_R^a$, $\widehat{\rho}_R^b$, ... for the sub-system quantum states that occur in any separable state is simply that these are possible quantum states of the sub-systems when the latter are considered as separate quantum systems before being combined as in the Werner protocol [7] to form the separable state. Hence all the justifications based either on simple physical considerations or phase reference systems that were previously invoked for the density operator $\widehat{\rho}$ of any general quantum states of the combined sub-systems to establish the *global particle number* SSR apply equally well here. No more need be said. It is contended that expressions for the non-entangled quantum state $\widehat{\rho}$ in which $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, $\widehat{\rho}_R^C$... were *not* allowed quantum 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* [54, 60] as one of several *operational approaches* for defining entangled states. As pointed out above other authors [56, 57] define separable (and hence entangled) states differently by specifically allowing sub-system density operators that are *not* consistent with the local particle number SSR, though the overall density operator is globally SSR consistent. The corresponding overall states are termed *separable but non-local*, and states that they would regard as separable would here be regarded as entangled. Examples of such states are given in equations (83) and (85). There are also other authors [61, 62] who define separable (and hence entangled) states via (3) but leave unspecified whether the sub-system density operators are consistent or inconsistent with the local particle number SSR. Note that any inequalities involving measured quantities that are found for separable states in which local SSR compliance is *neglected* must also apply to separable states where it is *required*. The consequent implications for entanglement tests where local particle number SSR compliance is required is discussed in the accompanying paper II. Hence, in this paper we are advocating a *revision* to a *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 SSRs on particle numbers be applied to the the *overall* quantum 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 have been discussed above—basically it is because in separable states the sub-system density operators must represent possible quantum states for the sub-systems considered as isolate quantum systems, so the general reasons for applying the SSR will apply to these density operators also. Apart from the papers by Bartlett *et al* [54, 60] we are not aware that this definition of non-entangled states has been invoked previously, indeed the opposite approach has been proposed [56, 57]. However, the idea of considering whether sub-system states should satisfy the local particle number SSR has been presented in several papers—[54, 56, 57, 60, 63–65], 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 [56], multicopy distillation [54], mechanical work and accessible entanglement [63, 64] and Bell inequality violation [65]. 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. These tests are also discussed in the accompanying paper II.

3.4.2. Global but not local particle number SSR compliant states. There is a connection between global SSR compliance for separable states in general and local SSR

compliance for the component sub-system states. This may be stated in the form of a theorem:

Theorem. *A necessary and sufficient condition for all separable states for a given set of sub-system density operators* $\widehat{\rho}_R^a$, $\widehat{\rho}_R^b$ *to be global particle number SSR compliant is that all such sub-system states are local particle number SSR compliant.*

The proof of this theorem is set out in appendix N. It deals with the case where the probabilities P_R for preparing a particular product $\widehat{\rho}_R^A \otimes \widehat{\rho}_R^B$ of sub-system states in the Werner process can be arbitrarily varied. The theorem shows that in general global and local SSR compliance always occur together in separable states.

However, it should be noted that some authors [56, 57] consider sub-system density operators in the context of two mode systems which comply with the global particle number SSR but not the local particle number SSR. These involve special choices of both the sub-system states and the product preparation probabilities. Such a case involving four *zero and one boson superpositions* is presented by Verstraete *et al* [56, 57]. The overall density operator is a statistical mixture

$$\begin{aligned}\widehat{\rho} = &\frac{1}{4}(|\psi_1\rangle\langle\psi_1|)_A \otimes |\psi_1\rangle\langle\psi_1|)_B \\ &+ \frac{1}{4}(|\psi_i\rangle\langle\psi_i|)_A \otimes |\psi_i\rangle\langle\psi_i|)_B \\ &+ \frac{1}{4}(|\psi_{-1}\rangle\langle\psi_{-1}|)_A \otimes |\psi_{-1}\rangle\langle\psi_{-1}|)_B \\ &+ \frac{1}{4}(|\psi_{-i}\rangle\langle\psi_{-i}|)_A \otimes |\psi_{-i}\rangle\langle\psi_{-i}|)_B, \end{aligned} \tag{83}$$

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 $|\psi_\omega\rangle\langle\psi_\omega|)_B$. Although the expression in equation (83) is of the form in equation (3), the subsystem density operators $|\psi_\omega\rangle\langle\psi_\omega|)_A$ and $|\psi_\omega\rangle\langle\psi_\omega|)_B$ do not comply with the local particle number SSR, so in the present paper and in [5] the state would be regarded as *entangled*. However, Verstraete *et al* [56, 57] regard it as separable. They refer to such a state as *separable but non-local*.

On the other hand, the global particle number SSR is obeyed since the density operator can also be written as

$$\begin{aligned}\widehat{\rho} = &\frac{1}{4}(|0\rangle\langle 0|)_A \otimes |0\rangle\langle 0|)_B + \frac{1}{4}(|1\rangle\langle 1|)_A \otimes |1\rangle\langle 1|)_B \\ &+ \frac{1}{2}(|\Psi_+\rangle\langle\Psi_+|)_{AB}, \end{aligned} \tag{84}$$

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. Note that equation (84) 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.

To further illustrate some of the points made about SSRs —local and global—it is useful to consider a second specific case also presented by Verstraete *et al* [56, 57]. This *mixture* of *two mode coherent states* is represented by the two mode density operator

$$\begin{aligned}\widehat{\rho} &= \int \frac{\mathrm{d}\theta}{2\pi}|\alpha,\, \alpha\rangle\langle\alpha,\, \alpha| \\ &= \int \frac{\mathrm{d}\theta}{2\pi}(|\alpha\rangle\langle\alpha|)_A \otimes (|\alpha\rangle\langle\alpha|)_B, \end{aligned} \tag{85}$$

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

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

$$\widehat{\rho} = \sum_R P_R\, \widehat{\rho}_R^A \otimes \widehat{\rho}_R^B \tag{86}$$

with $\sum_R P_R \to \int \frac{\mathrm{d}\theta}{2\pi}$ and $\widehat{\rho}_R^A \to (|\alpha\rangle\langle\alpha|)_A$ and $\widehat{\rho}_R^B \to (|\alpha\rangle\langle\alpha|)_B$. However although this choice of $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$ satisfy the Hermitiancy, unit trace, positivity features they do *not* conform to the requirement of satisfying the (*local*) sub-system boson number SSR. From equation (85) we have

$$\begin{aligned}\langle n|(|\alpha\rangle\langle\alpha|)\ |m\rangle_A &= \exp(-|\alpha|^2)\frac{\alpha^n}{\sqrt{n!}}\frac{(\alpha)^{*m}}{\sqrt{m!}} \\ \langle p|(|\alpha\rangle\langle\alpha|)\ |q\rangle_B &= \exp(-|\alpha|^2)\frac{\alpha^p}{\sqrt{p!}}\frac{(\alpha)^{*q}}{\sqrt{q!}} \end{aligned} \tag{87}$$

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 equation (85) does *not* represent a non-entangled state. However, in the papers of Verstraete *et al* [56, 57], Hillery *et al* [61, 62] and others it would represent an allowable non-entangled (separable) state. Indeed, Verstraete *et al* [56] specifically state '..., this state is *obviously* separable, though the states $|\alpha\rangle$ are incompatible with the (local) super-selection rule'. Verstraete *et al* [56] introduce the state defined in equation (85) 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 SSR.

The *mixture* of *two mode coherent states* does of course satisfy the *total* or *global* boson number SSR. The matrix elements between two mode Fock states are

$$\begin{aligned}&(\langle n|_A \otimes \langle p|_B)\widehat{\rho}(|m\rangle_A \otimes |q\rangle_B) \\ &= \exp(-2|\alpha|^2)\frac{|\alpha|^{n+m}}{\sqrt{n!}\sqrt{m!}}\frac{|\alpha|^{p+q}}{\sqrt{p!}\sqrt{q!}}\int\frac{\mathrm{d}\theta}{2\pi} \\ &\quad\times\exp(-\mathrm{i}(n-m+p-q)\theta) \\ &= \exp(-2|\alpha|^2)\frac{|\alpha|^{n+m}}{\sqrt{n!}\sqrt{m!}}\frac{|\alpha|^{p+q}}{\sqrt{p!}\sqrt{q!}}\,\delta_{n+p,m+q}. \end{aligned} \tag{88}$$

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 SSR.

The *reduced density operators* for modes A, B are

$$\widehat{\rho}_A = \int \frac{\mathrm{d}\theta}{2\pi}(|\alpha\rangle\langle\alpha|)_A \qquad \widehat{\rho}_B = \int \frac{\mathrm{d}\theta}{2\pi}(|\alpha\rangle\langle\alpha|)_B$$

and a straightforward calculation gives

$$\widehat{\rho}_A = \exp(-|\alpha|^2)\sum_n \frac{|\alpha|^{2n}}{n!}(|n\rangle\langle n|)_A$$
$$\widehat{\rho}_B = \exp(-|\alpha|^2)\sum_p \frac{|\alpha|^{2p}}{p!}(|p\rangle\langle p|)_B$$

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 SSR, whereas the density operators $\widehat{\rho}_R^A = (|\alpha\rangle\langle\alpha|)_A$, $\widehat{\rho}_R^B = (|\alpha\rangle\langle\alpha|)_B$ are *not*. Later we will revisit this example in the context of entanglement tests.

Note that if a twirling operation (see appendix equation (263)) 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.

3.4.3. General form of non-entangled states. To summarize: basically the sub-systems are *single modes* that the identical bosons can occupy, the SSR for identical bosons, massive or otherwise, prohibits states which are coherent superpositions of states with different numbers of bosons, and the only physically allowable $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, ... 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

$$\widehat{\rho}_R^A = \sum_{n_A} P_{n_A}^A |n_A\rangle\langle n_A| \quad \widehat{\rho}_R^B = \sum_{n_B} P_{n_B}^B |n_B\rangle\langle n_B| \ldots \tag{89}$$

However, in cases where the sub-systems are *pairs of modes* the density operators $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, ... for the separate sub-systems are still required to conform to the symmetrization principle and the SSR. The forms for $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, ... 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 equation (3) 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 equation (64). We have

$$|\Phi_{N_A}\rangle_A = \sum_{k=0}^{N_A} C_{A\Phi}(N_A, k)|k\rangle_{A_1} \otimes |N_A - k\rangle_{A_2}$$
$$\widehat{\rho}_R^A = \sum_{N_A=0}^{\infty}\sum_{\Phi} P_{\Phi N_A}|\Phi_{N_A}\rangle_A\langle\Phi_{N_A}|_A \tag{90}$$

with analogous expressions for the density operators $\widehat{\rho}_R^B$ 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 (248) in appendix D of paper II is of this form.

3.5. Bipartite systems

We now consider the bipartite case where there are just two sub-systems involved. The simplest case is where each sub-system involves only a single mode, such as for two modes in a double well potential when only a single hyperfine state is involve. Another important case is where each sub-system contains two modes, such as in the double well case where modes with two different hyperfine states are involved.

3.5.1. Two single modes—coherence terms. The general non-entangled state for modes $\widehat{a}$ and $\widehat{b}$ is given by

$$\widehat{\rho} = \sum_R P_R\, \widehat{\rho}_R^A \otimes \widehat{\rho}_R^B \tag{91}$$

and as a consequence of the requirement that $\widehat{\rho}_R^A$ and $\widehat{\rho}_R^B$ are allowed quantum states for modes $\widehat{a}$ and $\widehat{b}$ satisfying the SSR, it follows that

$$\langle(\widehat{a})^n\rangle_a = \mathrm{Tr}(\widehat{\rho}_R^A(\widehat{a})^n) = 0$$
$$\langle(\widehat{a}^\dagger)^n\rangle_a = \mathrm{Tr}(\widehat{\rho}_R^A(\widehat{a}^\dagger)^n) = 0$$
$$\langle(\widehat{b})^m\rangle_b = \mathrm{Tr}(\widehat{\rho}_R^B(\widehat{b})^m) = 0$$
$$\langle(\widehat{b}^\dagger)^m\rangle_b = \mathrm{Tr}(\widehat{\rho}_R^B(\widehat{b}^\dagger)^m) = 0. \tag{92}$$

Thus coherence terms are zero. As we will see these results will limit spin squeezing to entangled states of modes $\widehat{a}$ and $\widehat{b}$. Note that similar results also apply when non-entangled states for the original modes $\widehat{c}$ and $\widehat{d}$ are considered- $\langle(\widehat{c})^n\rangle_c = 0$, etc.

3.5.2. Two pairs of modes—coherence terms. In this case the general non-entangled state where A and B are pairs of modes —$\widehat{a}_1$, $\widehat{a}_2$ associated with sub-system A, and modes $\widehat{b}_1$, $\widehat{b}_2$ associated with sub-system B, the overall density operator is of the form (91). Consistent with the requirement that the sub-system density operators $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$ conform to the symmetrization principle and the SSR, these density operators will *not* in general represent separable states for their single mode sub-systems $\widehat{a}_1$, $\widehat{a}_2$ or $\widehat{b}_1$, $\widehat{b}_2$—and may even be entangled states. As a result when considering *non-entangled* states for the sub-systems A and B we now have

$$\langle(\widehat{a}_i^\dagger\widehat{a}_j)^n\rangle_A = \mathrm{Tr}(\widehat{\rho}_R^A(\widehat{a}_i^\dagger\widehat{a}_j)^n) \neq 0 \quad i,j = 1,2$$
$$\langle(\widehat{b}_i^\dagger\widehat{b}_j)^n\rangle_A = \mathrm{Tr}(\widehat{\rho}_R^B(\widehat{b}_i^\dagger\widehat{b}_j)^n) \neq 0 \quad i,j = 1,2 \tag{93}$$

in general. In this case where the sub-systems are *pairs* of modes the spin squeezing entanglement tests as in equations (37)–(39) in paper II for sub-systems consisting of *single* modes cannot be applied, as we will see. Nevertheless, there are still tests of bipartite entanglement involving spin operators.

4. Discussion and summary of key results

This paper is mainly concerned with two mode entanglement for systems of identical massive bosons, though multimode entanglement is also considered. These bosons may be atoms or molecules as in cold quantum gases. In the present paper we focus on the definition and general features of entanglement, while in the accompanying paper we consider spin squeezing and other tests for entanglement.

The present paper starts with the *general definition* of *entanglement* for a system consisting of several *sub-systems*, and highlights the distinctive *features* of entangled states in regard to measurement probabilities for joint measurements on the sub-systems in contrast to the results for non-entangled or *separable* states. The relationship between entanglement and HVT is then explored followed by a discussion of key *paradoxes* such as EPR and violations of Bell inequalities. The notion of entanglement *measures* and entanglement *tests* was briefly introduced, the latter being covered more fully in the accompanying paper II [6].

The paper then focuses on entanglement for systems of identical massive particles in the regime of non-relativistic quantum physics. 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 quantum states, not as differing physical systems, and the *symmetrization principle* required of quantum states for identical particle systems will be satisfied by using Fock states to describe the states.

Furthermore, it is argued that the overall quantum states should conform to the superselection rule that excludes quantum superposition states of the form (61) as allowed quantum 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 for massive bosons, which may be summarized 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; and (3) There is no need to invoke the existence of such states in order to understand coherence and interference effects. Invoking the 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 SSRs, *this paper differs* from a number of others by *extending* the SSR to also apply to the density operators $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, ... for the *mode sub-systems* A, B, ... that occur in the definition (3) 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 $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, ... 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* SSR 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 SSR 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 (23) for these measurements depends on all the density operators $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, ... for the mode sub-systems as well as the probability P_R for the product state $\widehat{\rho}_R^A \otimes \widehat{\rho}_R^B \otimes \ \ldots$ occurring when the general mixed non-entangled state is prepared, which can be accomplished by local preparations and classical communication. For the non-entangled state the form of the joint probability $P_{AB\ldots}(i, j, \ldots)$ for measurements on all the sub-systems is given by the products of the individual sub-system probabilities $P_A^R(i) = \mathrm{Tr}(\widehat{\Pi}_i^A \, \widehat{\rho}_R^A)$, etc that measurements on the sub-systems A, B, … yield the outcomes λ_i^A etc when the sub-systems are in states $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, ..., the overall products being weighted by the probability P_R that a particular product state is prepared. If $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, ... did not represent allowed quantum states then the interpretation of the joint probability as this statistical average would be unphysical. Thirdly, attempts to allow the density operators $\widehat{\rho}_R^A$, $\widehat{\rho}_R^B$, ... for the mode sub-systems to violate the SSR provided that the reduced density operators $\widehat{\rho}_A$, $\widehat{\rho}_B$ 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 SSR 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 K 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.

In regard to entanglement measures, we discussed the particle entanglement measure of Wiseman *et al* [45, 46] and found that a non-zero result for the particle entanglement measure *shows* that the state must be *entangled.* However, as for other entanglement measures the problem with using the particle entanglement measure to detect entangled states is that there is no obvious way to measure it experimentally. On the other hand, as will be seen in the accompanying paper II, the quantities involved in entanglement tests can be measured experimentally.

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Appendix

The following appendices can be found in the supplementary data here (stacks.iop.org/ps/92/023004/mmedia)

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Discussions of the cited articles [108–122] can be found within the supplementary data here stacks.iop.org/ps/92/023004/mmedia.

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