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QUANTUM ENTANGLEMENT FOR SYSTEMS OF IDENTICAL BOSONS

I. GENERAL FEATURES:

APPENDICES

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Appendix A  Werner States

The mixed entangled states considered by Werner [7] for which a hidden variable theory could be constructed were of a special form. Two distinguishable subsystems each with $d$ basis states $|u_r\rangle$ were considered, for which the states could be transformed by unitary operators $\hat{U}$, and the combined density operator $\hat{\rho}$ was required to be invariant under all unitary transformations of the form $\hat{U} \otimes \hat{U}$, so that $\hat{\rho} = (\hat{U} \otimes \hat{U})\hat{\rho}(\hat{U}^\dagger \otimes \hat{U}^\dagger)$. Werner [7] considered the following unitary operators: (a) $\hat{U}_{-r}$ such that $\hat{U}_{-r} |u_r\rangle = -|u_r\rangle$, $\hat{U}_{-r} |u_s\rangle = +|u_s\rangle$ for $s \neq r$ (b) $\hat{P}(r \rightarrow \mu r)$, which permute basis states $\hat{P}(r \rightarrow \mu r) |u_r\rangle = |u_{\mu r}\rangle$ (c) $\hat{U}_{rot}(n, m)$, which transform basis states into linear combinations of each other $\hat{U}_{rot}(n, m) |u_n\rangle = U_{nn} |u_n\rangle + U_{nm} |u_m\rangle$, $\hat{U}_{rot}(n, m) |u_m\rangle = U_{mn} |u_n\rangle + U_{mm} |u_m\rangle$. As a consequence of these invariances Werner [7] showed that the density operator could be expressed in terms of a single parameter $\Phi$ in the form $\hat{\rho} = \left(d^3 - d \right)^{-1} \left\{ (d - \Phi)\hat{1} + (d\Phi - 1)\hat{V} \right\}$, where $\hat{1}$ is the unit operator and $\hat{V}$ is the flip operator. These have matrix elements $\left(\hat{1}\right)_{rs, nm} = \delta_{rn} \delta_{sm}$ and $\left(\hat{V}\right)_{rs, nm} = \delta_{rm} \delta_{sn}$. From this form of the density operator Werner [7] showed that the probability function for joint measurement outcomes on the two sub-systems could be expressed in the same form as applied in hidden variable theory. So although the mixed entangled state Werner considered were of a restricted type, the work demonstrated that entanglement did not preclude all hidden variable theory interpretations of the joint measurements. The fact that some entangled states do not violate a Bell inequality is another consequence of Werner’s result.

Appendix B  Classical Entanglement

In addition to quantum entanglement there is a body of work (see [108], [109], [100]) dealing with so-called classical entanglement. Here the states of classical systems - such as a classical EM field - are represented via a formalism involving linear vector spaces and classical entanglement is defined mathematically. A discussion of classical entanglement is beyond the scope of this paper. Although there are some formal similarities with quantum entanglement - and even Bell type inequalities which can be violated, there are key features that is not analogous to that for composite quantum systems - quantum non-locality being one [108]. In the end, rather than just focusing on similarities in the mathematical formalisms, classical and quantum entanglement are seen as fundamentally different when the physics of the two different types of system - one classical and deterministic, the other quantum and probabilistic are taken into account. In particular, the key feature of quantum entanglement relating to joint measurement probabilities is quite different to the corresponding one for classical entanglement.
Appendix C  Projective Measurements and Conditional Probabilities

C.1  Details on Conditional Probabilities

C.1.1  Projective Measurements

For simplicity, we will only consider projective (or von Neumann) measurements rather than more general measurements involving positive operator measurements (POM). If $\hat{\Omega}$ is a physical quantity associated with the system, with eigenvalues $\lambda_i$ and with $\hat{\Pi}_i$ the projector onto the subspace with eigenvalue $\lambda_i$, then the probability $P(i)$ that measurement of $\hat{\Omega}$ leads to the value $\lambda_i$ is given by [85]

$$P(i) = Tr(\hat{\Pi}_i \hat{\rho})$$  \hspace{1cm} (94)

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

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

$$\hat{\rho}_{\text{cond}}(\hat{\Omega}, i) = (\hat{\Pi}_i \hat{\rho} \hat{\Pi}_i) / P(i)$$  \hspace{1cm} (95)

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

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

$$\langle \hat{\Omega} \rangle_i = Tr(\hat{\Omega} \hat{\rho}_{\text{cond}}(\hat{\Omega}, i))$$
$$= Tr(\hat{\Omega} (\hat{\Pi}_i \hat{\rho} \hat{\Pi}_i)) / P(i)$$
$$= \lambda_i Tr(\hat{\Pi}_i \hat{\rho}) / P(i)$$
$$= \lambda_i$$  \hspace{1cm} (96)
whilst for the variance
\[
\langle \Delta \hat{\Omega}^2 \rangle_i = \text{Tr}((\hat{\Omega} - \langle \hat{\Omega} \rangle_i)^2 \hat{\rho}_{\text{cond}}(\hat{\Omega}, i)) = \text{Tr}(\hat{\Omega}^2 \hat{\rho}_{\text{red}}(i)) - \langle \hat{\Omega} \rangle_i^2 = \lambda_i^2 - \lambda_i^2 = 0
\]
which is zero as expected.

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

C.1.2 Conditional Probabilities

Suppose we follow the measurement of \(\hat{\Omega}\) resulting in eigenvalue \(\lambda_i\) with a measurement of \(\hat{\Lambda}\) resulting in eigenvalue \(\mu_j\) where the projector associated with the latter measurement is \(\hat{\Xi}_j\). Then the conditional probability of measuring \(\hat{\Lambda}\) resulting in eigenvalue \(\mu_j\) following the measurement of \(\hat{\Omega}\) that resulted in eigenvalue \(\lambda_i\) would be
\[
P(j|i) = \text{Tr}(\hat{\Xi}_j \hat{\Pi}_i \hat{\xi}) = \frac{\text{Tr}(\hat{\Xi}_j (\hat{\Pi}_i \hat{\rho} \hat{\Pi}_i))}{P(i)} = \frac{\text{Tr}((\hat{\Xi}_j \hat{\Pi}_i) \hat{\rho} (\hat{\Pi}_i \hat{\Xi}_j))}{P(i)}
\]
where the cyclic properties of the trace and the idempotent property of the projector have been used. If the measurements had taken place in the reverse order the conditional probability of measuring \(\hat{\Omega}\) resulting in eigenvalue \(\lambda_i\) following the measurement of \(\hat{\Lambda}\) that resulted in eigenvalue \(\mu_j\) would be
\[
P(i|j) = \text{Tr}((\hat{\Pi}_i \hat{\Xi}_j) \hat{\rho} (\hat{\Xi}_j \hat{\Pi}_i))/P(j)
\]

We note that the actual probability of measuring \(\lambda_i\) then \(\mu_j\) would be the joint probability
\[
P(j \text{ after } i) = P(j|i) P(i) = \text{Tr}((\hat{\Xi}_j \hat{\Pi}_i) \hat{\rho} (\hat{\Pi}_i \hat{\Xi}_j))
\]

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

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

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

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

$$P(i,j) = P(j|i) P(i) = P(i|j) P(j) = \text{Tr}((\hat{\Pi}_i \hat{\Xi}_j) \hat{\rho} (\hat{\Xi}_j \hat{\Pi}_i))$$

is an expression of Bayes theorem.

A case of particular importance where this occurs is in situations involving two or more distinct sub-systems, in which the operators $\hat{\Omega}$ and $\hat{\Lambda}$ are associated with different sub-systems. For two sub-systems $A$ and $B$ the operators $\hat{\Omega}$ and $\hat{\Lambda}$ are of the form $\hat{\Omega}_A$ and $\hat{\Omega}_B$, or more strictly $\hat{\Omega}_A \otimes \hat{1}_B$ and $\hat{1}_A \otimes \hat{\Omega}_B$. It is easy to see that $(\hat{\Omega}_A \otimes \hat{1}_B)(\hat{1}_A \otimes \hat{\Omega}_B) = \hat{\Omega}_A \otimes \hat{\Omega}_B = (\hat{1}_A \otimes \hat{\Omega}_B)(\hat{\Omega}_A \otimes \hat{1}_B)$, so the operators commute and results such as in Bayes theorem (103) apply.

### C.1.3 Conditional Mean and Variance

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

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

$$= \text{Tr}(\hat{\Lambda} (\hat{\Pi}_i \hat{\rho} \hat{\Pi}_i))/P(i)$$

(104)

Now

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

(105)

so that

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

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

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

(106)
using $\hat{\Xi}_j = \hat{\Xi}_2^j$, the cyclic trace properties and Eq.(99). Hence the conditional mean value is as expected, with the conditional probability $P(j|i)$ replacing $P(j)$ in the averaging process.

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

$$\langle \Delta \hat{\Lambda}^2 \rangle_i = Tr((\hat{\Lambda} - \langle \hat{\Lambda} \rangle_i)^2 \hat{\rho}_{\text{cond}}(\hat{\Omega}, i))/P(i) \quad (107)$$

Now

$$\langle \hat{\Lambda} - \langle \hat{\Lambda} \rangle_i \rangle^2 = \sum_j (\mu_j - \langle \hat{\Lambda} \rangle_i)^2 \hat{\Xi}_j \quad (108)$$

so that

$$\langle \Delta \hat{\Lambda}^2 \rangle_i = \sum_j (\mu_j - \langle \hat{\Lambda} \rangle_i)^2 Tr(\hat{\Xi}_j \hat{\Pi}_i \hat{\rho}_{\text{cond}}(\hat{\Omega}, i))/P(i) \quad (109)$$

using the same steps as for the conditioned mean. Hence the conditional variance is as expected, with the conditional probability $P(j|i)$ replacing $P(j)$ in the averaging process.

C.2 Detailed Inequalities for EPR Situation

For separable states the conditional probability that measurement of $\hat{p}_A$ on sub-system $A$ leads to eigenvalue $p_A$ given that measurement of $\hat{p}_B$ on sub-system $B$ leads to eigenvalue $p_B$ is obtained from Eq.(30) as

$$P(\hat{p}_A, p_A|\hat{p}_B, p_B) = \sum_R P_R P_A^R(\hat{p}_A, p_A) P_B^R(\hat{p}_B, p_B) / \sum_R P_R P_B^R(\hat{p}_B, p_B) \quad (110)$$

where

$$P_A^R(\hat{p}_A, p_A) = Tr_A(\hat{\Pi}_{p_A}^A \hat{\rho}_R^A) \quad P_B^R(\hat{p}_B, p_B) = Tr_B(\hat{\Pi}_{p_B}^B \hat{\rho}_R^B) \quad (111)$$

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

$$P(\hat{p}_B, p_B) = \sum_R P_R P_B^R(\hat{p}_B, p_B) \quad (112)$$

S 8
The mean result for measurement of $\hat{p}_A$ for this conditional measurement is from Eq.(19)

$$
\langle \hat{p}_A \rangle_{\hat{p}_B,p_B} = \sum_{p_A} p_A P(\hat{p}_A,p_A|\hat{p}_B,p_B)
$$

$$
= \sum_R P_R \langle \hat{p}_A \rangle_R P_R^R(\hat{p}_B,p_B)/P(\hat{p}_B,p_B)
$$

(113)

where

$$
\langle \hat{p}_A \rangle_R = \sum_{p_A} p_A P_A(\hat{p}_A,p_A)
$$

(114)

is the mean result for measurement of $\hat{p}_A$ when the sub-system is in state $\hat{\rho}_A$. The conditional variance for measurement of $\hat{p}_A$ for the conditional measurement of $\hat{p}_B$ on sub-system $B$ which led to eigenvalue $p_B$ is from Eq.(20)

$$
\langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_B,p_B} = \sum_{p_A} (p_A - \langle \hat{p}_A \rangle_{\hat{p}_B,p_B})^2 P(\hat{p}_A,p_A|\hat{p}_B,p_B)
$$

$$
= \sum_R P_R \langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A,p_a} P_R^R(\hat{p}_B,p_B)/P(\hat{p}_B,p_B)
$$

(115)

where

$$
\langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A,p_a} = \sum_{p_A} (p_A - \langle \hat{p}_A \rangle_{\hat{p}_B,p_B})^2 P_A(\hat{p}_A,p_A)
$$

is a variance for measurement of $\hat{p}_A$ for when the sub-system is in state $\hat{\rho}_A$ but now with the fluctuation about the mean $\langle \hat{p}_A \rangle_{\hat{p}_B,p_B}$ for measurements conditional on measuring $\hat{p}_B$.

However, for each sub-system state $R$ the quantity $\langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_B,p_B}^R$ is minimized if $\langle \hat{p}_A \rangle_{\hat{p}_B,p_B}$ is replaced by the unconditioned mean $\langle \hat{p}_A \rangle_R$ just determined from $\hat{\rho}_R$. Thus we have an inequality

$$
\langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_B,p_B}^R \geq \langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A}^R
$$

(116)

where

$$
\langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A}^R = \sum_{p_A} (p_A - \langle \hat{p}_A \rangle_{\hat{p}_B,p_B})^2 P_A(\hat{p}_A,p_A)
$$

(117)

is the normal variance for measurement of $\hat{p}_A$ for when the sub-system is in state $\hat{\rho}_R$.

Now if the measurements of $\hat{p}_B$ are unrecorded then the conditioned variance is

$$
\langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_B} = \sum_{x_B} \langle \Delta \hat{p}_A^2 \rangle_{\hat{x}_B,x_B} P(\hat{x}_B,x_B)
$$

$$
= \sum_{x_B} \sum_R P_R \langle \Delta \hat{p}_A^2 \rangle_{\hat{x}_B,x_B} P_R^R(\hat{x}_B,x_B)
$$

(118)
which in view of inequality (142) satisfies
\[
\langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A} \geq \sum_{\hat{p}_B} \sum_R P_R \langle \Delta \hat{p}_A^2 \rangle^R R^R_{\hat{p}_B, p_B} \\
= \sum_R P_R \langle \Delta \hat{p}_A^2 \rangle^R 
\]
using \( \sum_{\hat{p}_B} P^R_{\hat{p}_B, p_B} = 1 \). Thus the variance for measurement of momentum \( \hat{p}_A \) conditioned on unrecorded measurements for momentum \( \hat{p}_B \) satisfies an inequality that only depends on the variances for measurements of \( \hat{p}_A \) in the possible sub-system \( A \) states \( \hat{\rho}_R^A \).
Appendix D  LHV Violation in the GHZ State

The GHZ state [90], [91] is an entangled state of three sub-systems A, B and C, each of which is associated with two quantum states |+1⟩ and |−1⟩. Each sub-system has three physical quantities, which correspond to Pauli spin operators \( \hat{\sigma}_x, \hat{\sigma}_y \) and \( \hat{\sigma}_z \). The quantum states |+1⟩ and |−1⟩ are eigenstates of \( \hat{\sigma}_z \) with eigenvalues +1 and −1 respectively. Note that the eigenvalues of the other two Pauli spin operators are also +1 and −1. The GHZ state is defined by

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

(120)

The GHZ state provides a clear example of an entangled quantum state which cannot be described via local hidden variable theory [91], [92]. In a non-fuzzy version of the LHV model each of the nine physical quantities \( \sigma^x_A, \sigma^y_A, \sigma^z_A, \sigma^x_y, \sigma^y_y, \sigma^z_y, \sigma^x_z, \sigma^y_z, \sigma^z_z \) will be associated with hidden variables that directly specify the values +1 and −1 that each one of these physical quantities may have. We denote these hidden variables as \( M^K \), where \( K = A, B, C \) and \( \alpha = x, y, z \) and we have \( M^K = +1 \) or −1. With this direct specification of the physical values Eq. (35) just becomes \( \langle \sigma^K(M^K) \rangle = M^K \) and Eq. (36) becomes

\[
\langle \sigma^x_A \times \sigma^y_B \times \sigma^z_C \rangle_{LHV} = M^K M_B M_C
\]

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

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

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

(121)

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

\[
\hat{\sigma}_x^A \hat{\sigma}_y^B \hat{\sigma}_y^C |\Psi\rangle_{GHZ} = (−1) |\Psi\rangle_{GHZ}
\]

\[
\hat{\sigma}_y^A \hat{\sigma}_z^B \hat{\sigma}_y^C |\Psi\rangle_{GHZ} = (−1) |\Psi\rangle_{GHZ}
\]

\[
\hat{\sigma}_y^A \hat{\sigma}_z^B \hat{\sigma}_z^C |\Psi\rangle_{GHZ} = (−1) |\Psi\rangle_{GHZ}
\]

(122)

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

\[
M^A_x M^B_y M^C_z = −1 \quad M^A_y M^B_x M^C_z = −1 \quad M^A_y M^B_y M^C_x = −1
\]

(123)

Secondly, if we apply all three operators \( \hat{\sigma}_x^A \hat{\sigma}_y^B \hat{\sigma}_x^C \) to the GHZ state we find another eigenvalue equation

\[
\hat{\sigma}_x^A \hat{\sigma}_y^B \hat{\sigma}_x^C |\Psi\rangle_{GHZ} = (−1) |\Psi\rangle_{GHZ}
\]

(124)

which leads to

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

(125)
However, if we multiply the three equations in Eq. (123) together and use $(M^K) = +1$ we find that $M_x^A M_x^B M_x^C = -1$, in direct contradiction to the last equation. Thus the assignment of hidden variables for all the physical quantities $\alpha^K$ fails to describe the GHZ state. As we will see in the next SubSection, there are tests involving the violation of Bell Inequalities that are satisfied by some entangled states which allow a demonstration of the failure of more general local LHV theories, even allowing for correlations that are less than ideal.

The assumption of non-fuzzy LHV theories is not essential for the GHZ argument in the case of the ideal GHZ state (120). This is because one may use the correlations of (122) to establish a precise prediction of one of the spins at $A$, by measuring the spins at the other two locations. The assumption of local realism (on which the LHV theory is based) then establishes a precise value for the hidden variable [90], [91], [92]. In a more realistic scenario where the GHZ correlations are not perfect, the “elements of reality” established this way become fuzzy, and in that case Mermin’s Bell inequality [92] can be used to establish a contradiction with LHV models.
Appendix E  Inequalities

These inequalities are examples of Cauchy-Schwarz inequalities.

E.1  Integral Inequality

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

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

(126)

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

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

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

$$= \int d\lambda P(\lambda)^2 C(\lambda)D(\lambda) + \int \int d\lambda d\mu (1 - \delta(\lambda - \mu)) P(\lambda)P(\mu) C(\lambda)D(\mu)$$

(127)

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

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

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

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

(128)

so that

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

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

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

$$\geq 0$$

(129)

which proves the result.

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

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

(130)

E.2  Sum Inequality

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

$$\sum_R P_R C_R \sum_R P_R D_R \geq \left( \sum_R P_R \sqrt{C_R D_R} \right)^2$$

(131)
To prove this write \( x = \sum_R P_R C_R \) and \( y = \sum_R P_R D_R \) Then

\[
xy = \sum_R P_R C_R \sum_S P_S D_S = \sum_R \sum_S P_R P_S C_R D_S = \sum_R P_R^2 C_R D_R + \sum_R \sum_S (1 - \delta_{RS}) P_R P_S C_R D_S \tag{132}
\]

Also, write \( z = \left( \sum_R P_R \sqrt{C_R D_R} \right)^2 \). Then

\[
z = \left( \sum_R P_R \sqrt{C_R D_R} \right) \left( \sum_S P_S \sqrt{C_S D_S} \right) = \sum_R \sum_S P_R P_S \sqrt{C_R D_R \cdot C_S D_S} = \sum_R P_R^2 C_R D_R + \sum_R \sum_S (1 - \delta_{RS}) P_R P_S \sqrt{C_R D_R \cdot C_S D_S} \tag{133}
\]

so that

\[
xy - z = \sum_R \sum_S P_R P_S (1 - \delta_{RS}) \left( C_R D_S - \sqrt{C_R D_R \cdot C_S D_S} \right) = \frac{1}{2} \sum_R \sum_S P_R P_S (1 - \delta_{RS}) \left( C_R D_S + C_S D_R - 2 \sqrt{C_R D_R \cdot C_S D_S} \right) = \frac{1}{2} \sum_R \sum_S P_S P_R (1 - \delta_{RS}) \left( \sqrt{C_R D_S} - \sqrt{C_S D_R} \right)^2 \geq 0 \tag{134}
\]

which proves the result.

For the special case where \( D_R = 1 \) and where \( \sum_R P_R = 1 \) we get the simpler result

\[
\sum_R P_R C_R \geq \left( \sum_R P_R \sqrt{C_R} \right)^2 \tag{135}
\]

This inequality is used in [61].
Appendix F  EPR Paradoxes

In this Appendix we present detailed proofs regarding the EPR paradoxes in the case of two subsystems, both for position and momentum and for different spin components.

F.1 Position-Momentum EPR Paradox

Here we will show that for separable states the products of the conditional variances \( \langle \Delta \hat{x}^2_A | \hat{x}_B \rangle \) and \( \langle \Delta \hat{p}^2_A | \hat{p}_B \rangle \) is always greater than or equal to \( \frac{1}{4} \hbar^2 \), showing that if the Heisenberg uncertainty principle is violated then the state must be entangled.

For separable states the conditional probability that measurement of \( \hat{x}_A \) on sub-system \( A \) leads to eigenvalue \( x_A \) given that measurement of \( \hat{x}_B \) on sub-system \( B \) leads to eigenvalue \( x_B \) is obtained from Eq. (30) as

\[
P(\hat{x}_A, x_A | \hat{x}_B, x_B) = \frac{\sum_R P_R P_A^R(\hat{x}_A, x_A) \rho_{AB}^B(\hat{x}_B, x_B)}{\sum_R P_R \rho_{AB}^B(\hat{x}_B, x_B)}
\]

where

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

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

\[
P(\hat{x}_B, x_B) = \sum_R P_R \rho_{AB}^B(\hat{x}_B, x_B)
\]

The mean result for measurement of \( \hat{x}_A \) for this conditional measurement is from Eq. (19)

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

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

where

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

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

The conditional variance for measurement of \( \hat{x}_A \) for the conditional measurement of \( \hat{x}_B \) on sub-system \( B \) which led to eigenvalue \( x_B \) is from Eq. (20)

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

\[
= \sum_R \langle \Delta \hat{x}^2_A \rangle_{\hat{x}_B, x_B} P_B^R(\hat{x}_B, x_B) / P(\hat{x}_B, x_B)
\]
where

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

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

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

\[ \langle \Delta \hat{x}_A^2 \rangle^R_{\overline{x}_B,x_B} \geq \langle \Delta \hat{x}_A^2 \rangle^R \]  
(142)

where

\[ \langle \Delta \hat{x}_A^2 \rangle^R = \sum_{x_A} (x_A - \langle \hat{x}_A \rangle)^2 P_A^R(\hat{x}_A,x_A) \]  
(143)

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

Now if the measurements of \( \hat{x}_B \) are unrecorded - as would be the case from the point of view of the experimenter on spatially well-separated sub-system \( A \) when measurements on this sub-system take place at the same time - then the conditioned variance is

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

\[ = \sum_{x_B} \sum_{x_A} P_R \langle \Delta \hat{x}_A^2 \rangle^R_{\overline{x}_B,x_B} P_B^R(\hat{x}_B,x_B) \]  
(144)

which in view of inequality (142) satisfies

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

\[ = \sum_{x_B} P_R \langle \Delta \hat{x}_A^2 \rangle^R \]  
(145)

using \( \sum_{x_B} P_B^R(\hat{x}_B,x_B) = 1 \). Thus the variance for measurement of position \( \hat{x}_A \) conditioned on unrecorded measurements for position \( \hat{x}_B \) satisfies an inequality that only depends on the variances for measurements of \( \hat{x}_A \) in the possible sub-system \( A \) states \( \hat{\rho}_A^R \).

Now exactly the same treatment can be carried out for the variance of momentum \( \hat{p}_A \) also conditioned on unrecorded measurements of measurements for
momentum $\hat{x}_B$. Details are given in Appendix C. We have with

$$\langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A} = \sum_{p_B} \langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A,p_B} P(\hat{p}_B,p_B)$$

$$\langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A,p_B} = \sum_{p_A} (p_A - \langle \hat{p}_A \rangle_{\hat{p}_A,p_B})^2 P(\hat{p}_A,p_A|\hat{p}_B,p_B)$$

$$\langle \hat{p}_A \rangle_{\hat{p}_A,p_B} = \sum_{p_A} p_A P(\hat{p}_A,p_A|\hat{p}_B,p_B)$$

the inequality

$$\langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A} \geq \sum_{R} P_R \langle \Delta \hat{p}_A^2 \rangle^R_{R}$$

with

$$\langle \Delta \hat{p}_A^2 \rangle^R = \sum_{p_A} (p_A - \langle \hat{p}_A \rangle)^2 P^R_A(\hat{p}_A)p_A$$

is the normal variance for measurement of $\hat{p}_A$ for when the sub-system is in state $\hat{p}_A^R$.

We now multiply the two conditional variances, which it is important to note were associated with two different conditioned states based on two different measurements - position and momentum - carried out on sub-system $B$.

$$\langle \Delta \hat{x}_A^2 \rangle_{\hat{x}_A} \langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A} \geq \sum_{R} P_R \langle \Delta \hat{x}_A^2 \rangle^R_{R} \sum_{S} P_S \langle \Delta \hat{p}_A^2 \rangle^S_{S}$$

However, from the general inequality given in Appendix E as Eq. (131)

$$\sum_{R} P_R C_R \sum_{R} P_R D_R \geq \left( \sum_{R} P_R \sqrt{C_R D_R} \right)^2$$

we then have

$$\langle \Delta \hat{x}_A^2 \rangle_{\hat{x}_A} \langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A} \geq \left( \sum_{R} P_R \sqrt{\langle \Delta \hat{x}_A^2 \rangle^R_{R} \langle \Delta \hat{p}_A^2 \rangle^R_{R}} \right)^2 \geq \left( \sum_{R} P_R \sqrt{\langle \Delta \hat{x}_A^2 \rangle^R_{R} \times \langle \Delta \hat{p}_A^2 \rangle^R_{R}} \right)^2$$

But we know from the HUP that for any given state $\hat{p}_A^R$ that $\langle \Delta \hat{x}_A^2 \rangle^R \langle \Delta \hat{p}_A^2 \rangle^R \geq \frac{1}{\hbar^2}$, so for the conditioned variances associated with a separable state $\langle \Delta \hat{x}_A^2 \rangle_{\hat{x}_A} \langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A} \geq \frac{1}{\hbar^2}$ showing that for a separable state the conditioned variances $\langle \Delta \hat{x}_A^2 \rangle_{\hat{x}_A} \langle \Delta \hat{p}_A^2 \rangle_{\hat{p}_A}$ still satisfy the HUP. It is important to note that these variances were associated with two different conditioned states based on two different measurements - position and momentum - carried out on sub-system $B$, the results of which the observer for sub-system $A$ would be unaware of. Thus if the EPR violations as defined in Eq. (37) are to occur then the state must be entangled.
F.2 Spin EPR Paradox

Here we describe the EPR paradox that Bohm [93] described for sub-systems 1 and 2 each of which has as observables three spin components $\hat{S}_{\alpha 1}$ and $\hat{S}_{\alpha 2}$ with $\alpha = x, y, z$. From (38), different spin components for each sub-system do not have simultaneous precise measurements leading to Heisenberg Uncertainty principle relations involving the variances and mean values

$$\left\langle \Delta \hat{S}_{\alpha 1}^2 \right\rangle \left\langle \Delta \hat{S}_{\beta 1}^2 \right\rangle \geq \frac{1}{4} \left| \left\langle \hat{S}_{\alpha 1} \right\rangle \right|^2 \quad \left\langle \Delta \hat{S}_{\alpha 2}^2 \right\rangle \left\langle \Delta \hat{S}_{\beta 2}^2 \right\rangle \geq \frac{1}{4} \left| \left\langle \hat{S}_{\alpha 2} \right\rangle \right|^2 \quad (152)$$

As in the case of position and momentum a special state of the combined system has interesting features. For the case where the spin quantum number of each sub-system is 1/2 the measured values for any spin component of either system is either +1/2 or −1/2. In terms of eigenstates for $\hat{S}_{x 1}$ and $\hat{S}_{x 2}$ we consider the state

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}} (|x, +\rangle_1 \otimes |x, -\rangle_2 - |x, -\rangle_1 \otimes |x, +\rangle_2) \quad (153)$$

This is actually one of the Bell states. In this form it shows that measurements of the $x$ components of the spins are perfectly correlated, so that for example if the measurement of $\hat{S}_{x 2}$ for sub-system 2 results in the value $-1/2$, then a subsequent measurement of $\hat{S}_{x 1}$ for sub-system 1 must result in the value $+1/2$. However, the same state can be expressed in terms of eigenstates for $\hat{S}_{y 1}$ and $\hat{S}_{y 2}$ as

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}} (|y, +\rangle_1 \otimes |y, -\rangle_2 - |y, -\rangle_1 \otimes |y, +\rangle_2) \quad (154)$$

and analogous statements regarding measurement correlations apply if the measurements were for $\hat{S}_{y 2}$ on sub-system 2 with a subsequent measurement of $\hat{S}_{y 1}$ on sub-system 1. If the two sub-systems were well-separated it might be expected that first measuring $\hat{S}_{x 2}$ for sub-system 2 would determine the result of measuring $\hat{S}_{x 1}$ for sub-system 1, and then measuring $\hat{S}_{y 2}$ for sub-system 2 would determine the result of measuring $\hat{S}_{y 1}$ for sub-system 1 - and as the second ($\hat{S}_{y 2}$) measurement on far distant sub-system 2 should not affect the former measurement on sub-system 1 this would appear to result in precise measured values for $\hat{S}_{x 1}$ and $\hat{S}_{y 1}$ on sub-system 1, which conflicts with the Heisenberg Uncertainty principle requirement that $\left\langle \Delta \hat{S}_{x 1}^2 \right\rangle \left\langle \Delta \hat{S}_{y 1}^2 \right\rangle \geq \frac{1}{4} \left| \left\langle \hat{S}_{x 1} \right\rangle \right|^2$.

However we can consider the variances for $\hat{S}_{x 1}$ and $\hat{S}_{y 1}$ which are conditional on measurements for $\hat{S}_{x 2}$ and $\hat{S}_{y 2}$ for sub-system 2 and show that for separable states of the two sub-systems we have

$$\left\langle \Delta \hat{S}_{x 1}^2 \right\rangle_{\hat{S}_{x 2}} \left\langle \Delta \hat{S}_{y 1}^2 \right\rangle_{\hat{S}_{y 2}} \geq \frac{1}{4} \left| \left\langle \hat{S}_{x 1} \right\rangle \right|^2 \quad (155)$$

Thus if we find that

$$\left\langle \Delta \hat{S}_{x 1}^2 \right\rangle_{\hat{S}_{x 2}} \left\langle \Delta \hat{S}_{y 1}^2 \right\rangle_{\hat{S}_{y 2}} < \frac{1}{4} \left| \left\langle \hat{S}_{x 1} \right\rangle \right|^2 \quad (156)$$
then we have an example of a spin EPR violation. Such a violation requires
that the quantum state is entangled.

F.2.1 Local Spin Operators

For two sub-systems 1 and 2 there are numerous possibilities for defining sep-
arrate commuting spin operators for the two systems. One situation of interest
is where each sub-system is associated with two bosonic modes, the standard
annihilation operators being $\hat{a}_1$ and $\hat{b}_1$ for system 1 and $\hat{a}_2$ and $\hat{b}_2$ for system 2.

The local spin operators for each sub-system can be defined as

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

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

(157)

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

$$
\hat{S}_\alpha = \hat{S}_\alpha^1 + \hat{S}_\alpha^2 \quad \alpha = x, y, z
$$

(158)

and these satisfy the usual angular momentum commutation rules.

F.2.2 Conditional Variances

The question is whether the conditional variances $\langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}}$ for measuring
$\hat{S}_{x1}$ for sub-system 1 having measured $\hat{S}_{x2}$ for sub-system 2, and $\langle \Delta \hat{S}_{y1}^2 \rangle_{\hat{P}_\alpha}$ for
measuring $\hat{S}_{y1}$ for sub-system 1 having measured $\hat{S}_{y2}$ for sub-system 2 violate
the Heisenberg Uncertainty Principle.

$$
\langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}} \langle \Delta \hat{S}_{y1}^2 \rangle_{\hat{P}_\alpha} < \frac{1}{4} |\langle \hat{S}_{z1} \rangle|^2
$$

(159)

where the measurements on sub-system 2 are left unrecorded. If this inequality holds we have an EPR violation.

For separable states the conditional probability that measurement of $\hat{S}_{x1}$ on
sub-system 1 leads to eigenvalue $s_{x1}$ given that measurement of $\hat{S}_{x2}$ on sub-
system 2 leads to eigenvalue $s_{x2}$ is obtained from Eq.(30) as

$$
P(\hat{S}_{x1}, s_{x1}|\hat{S}_{x2}, s_{x2}) = \sum_R P_R P_1^R(\hat{S}_{x1}, s_{x1}) P_2^R(\hat{S}_{x2}, s_{x2})/\sum_R P_R P_2^R(\hat{S}_{x2}, s_{x2})
$$

(160)

where

$$
P_1^R(\hat{S}_{x1}, s_{x1}) = Tr_1(\tilde{\Pi}_{s_{x1}} \tilde{\rho}_R^1) \quad P_2^R(\hat{S}_{x2}, s_{x2}) = Tr_2(\tilde{\Pi}_{s_{x2}} \tilde{\rho}_R^2)
$$

(161)
are the probabilities for spin measurements in the separate sub-systems. The probability that measurement of $\hat{S}_{x2}$ on sub-system 2 leads to eigenvalue $s_{x2}$ is

$$P(\hat{S}_{x2}, s_{x2}) = \sum_R P_R P^R_2(\hat{S}_{x2}, s_{x2})$$ (162)

The mean result for measurement of $\hat{S}_{x1}$ for this conditional measurement is from Eq.(19)

$$\langle \hat{S}_{x1} \rangle_{\hat{S}_{x2}, s_{x2}} = \sum_{s_{x1}} s_{x1} P(\hat{S}_{x1}, s_{x1} | \hat{S}_{x2}, s_{x2})$$

$$= \sum_R P_R \langle \hat{S}_{x1} \rangle_{R} P^R_2(\hat{S}_{x2}, s_{x2}) / P(\hat{S}_{x2}, s_{x2})$$ (163)

where

$$\langle \hat{S}_{x1} \rangle_{R} = \sum_{s_{x1}} s_{x1} P_R(\hat{S}_{x1}, s_{x1})$$ (164)

is the mean result for measurement of $\hat{S}_{x1}$ when the sub-system is in state $\hat{\rho}_R$.

The conditional variance for measurement of $\hat{S}_{x1}$ for the conditional measurement of $\hat{S}_{x2}$ on sub-system 2 which led to eigenvalue $s_{x2}$ is from Eq.(20)

$$\langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}, s_{x2}} = \sum_{s_{x1}} (s_{x1} - \langle \hat{S}_{x1} \rangle_{\hat{S}_{x2}, s_{x2}})^2 P(\hat{S}_{x1}, s_{x1} | \hat{S}_{x2}, s_{x2})$$

$$= \sum_R P_R \langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}, s_{x2}}^R P^R_2(\hat{S}_{x2}, s_{x2}) / P(\hat{S}_{x2}, s_{x2})$$ (165)

where

$$\langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}, s_{x2}}^R = \sum_{s_{x1}} (s_{x1} - \langle \hat{S}_{x1} \rangle_{\hat{S}_{x2}, s_{x2}})^2 P^R_1(\hat{S}_{x1}, s_{x1})$$

is a variance for measurement of $\hat{S}_{x1}$ for when the sub-system is in state $\hat{\rho}_R$, but now with the fluctuation about the mean $\langle \hat{S}_{x1} \rangle_{\hat{S}_{x2}, s_{x2}}$ for measurements conditional on measuring $\hat{S}_{x2}$.

However, for each sub-system state $R$ the quantity $\langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}, s_{x2}}^R$ is minimized if $\langle \hat{S}_{x1} \rangle_{\hat{S}_{x2}, s_{x2}}$ is replaced by the unconditioned mean $\langle \hat{S}_{x1} \rangle_{R}$ just determined from $\hat{\rho}_R$. Thus we have an inequality

$$\langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}, s_{x2}}^R \geq \langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x1}}^R$$ (166)

where

$$\langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x1}}^R = \sum_{s_{x1}} (s_{x1} - \langle \hat{S}_{x1} \rangle_{\hat{S}_{x1}})^2 P^R_1(\hat{S}_{x1}, s_{x1})$$ (167)
is the normal variance for measurement of $\hat{S}_{x1}$ for when the sub-system is in state $\hat{\rho}_R$.

Now if the measurements of $\hat{S}_{x2}$ are unrecorded - as would be the case from the point of view of the experimenter on spatially well-separated sub-system 1 when measurements on this sub-system take place at the same time - then the conditioned variance is

$$\langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}} = \sum_{s_{x2}} \langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}, s_{x2}} P(\hat{S}_{x2}, s_{x2})$$

$$= \sum_{s_{x2}} \sum_R P_R \langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}, s_{x2}}^R P^R_2(\hat{S}_{x2}, s_{x2})$$

which in view of inequality (142) satisfies

$$\langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}} \geq \sum_{s_{x2}} \sum_R P_R \langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}, s_{x2}}^R P^R_2(\hat{S}_{x2}, s_{x2})$$

which in view of inequality (142) satisfies

$$\langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}} \geq \sum_{s_{x2}} \sum_R P_R \langle \Delta \hat{S}_{x1}^2 \rangle_{\hat{S}_{x2}, s_{x2}}^R P^R_2(\hat{S}_{x2}, s_{x2})$$

using \( \sum_R P^R_2(\hat{S}_{x2}, s_{x2}) = 1 \). Thus the variance for measurement of spin $\hat{S}_{x1}$ conditioned on unrecorded measurements for spin $\hat{S}_{x2}$ satisfies an inequality that only depends on the variances for measurements of $\hat{S}_{x1}$ in the possible sub-system 1 states $\hat{\rho}_R$.

Now exactly the same treatment can be carried out for the variance of spin $\hat{S}_{y1}$ also conditioned on unrecorded measurements of measurements for momentum $\hat{S}_{y2}$. Details are given in Appendix C. We have with

$$\langle \Delta \hat{S}_{y1}^2 \rangle_{\hat{S}_{y2}} = \sum_{s_{y2}} \langle \Delta \hat{S}_{y1}^2 \rangle_{\hat{S}_{y2}, s_{y2}} P(\hat{S}_{y2}, s_{y2})$$

$$\langle \Delta \hat{S}_{y2}^2 \rangle_{\hat{S}_{y2}, s_{y2}} = \sum_{s_{y1}} (s_{y1} - \langle \hat{S}_{y1} \rangle_{\hat{S}_{y2}, s_{y2}})^2 P(\hat{S}_{y2}, s_{y2}|\hat{S}_{y2}, s_{y2})$$

$$\langle \hat{S}_{y1} \rangle_{\hat{S}_{y2}, s_{y2}} = \sum_{s_{y1}} s_{y1} P(\hat{S}_{y1}, s_{y1}|\hat{S}_{y2}, s_{y2})$$

the inequality

$$\langle \Delta \hat{S}_{y1}^2 \rangle_{\hat{S}_{y2}} \geq \sum_R P_R \langle \Delta \hat{S}_{y1}^2 \rangle_{\hat{S}_{y2}}^R$$

with

$$\langle \Delta \hat{S}_{y1}^2 \rangle_{\hat{S}_{y2}}^R = \sum_{s_{y1}} (s_{y1} - \langle \hat{S}_{y1} \rangle_{\hat{S}_{y2}})^2 P^R_1(\hat{S}_{y1}, s_{y1})$$

is the normal variance for measurement of $\hat{S}_{y1}$ for when the sub-system is in state $\hat{\rho}_R$. 

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We now multiply the two conditional variances, which it is important to note were associated with two different conditioned states based on two different measurements - spin $\hat{S}_{x2}$ and spin $\hat{S}_{y2}$ - carried out on sub-system 2.

$$\langle \Delta \hat{S}_{x1}^2 \rangle_{\tilde{S}_{x2}} \langle \Delta \hat{S}_{y1}^2 \rangle_{\tilde{S}_{y2}} \geq \sum_R P_R \langle \Delta \hat{S}_{x1}^2 \rangle_R \sum_S P_S \langle \Delta \hat{S}_{y1}^2 \rangle_S$$  \hspace{1cm} (172)

However, from the general inequality in Eq.(131)

$$\sum_R P_R C_R \sum_R P_R D_R \geq \left( \sum_R P_R \sqrt{C_R D_R} \right)^2$$  \hspace{1cm} (173)

we then have

$$\langle \Delta \hat{S}_{x1}^2 \rangle_{\tilde{S}_{x2}} \langle \Delta \hat{S}_{y1}^2 \rangle_{\tilde{S}_{y2}} \geq \left( \sum_R P_R \sqrt{\langle \Delta \hat{S}_{x1}^2 \rangle_R \langle \Delta \hat{S}_{y1}^2 \rangle_R} \right)^2$$  \hspace{1cm} (174)

But we know from the HUP that for any given state $\tilde{\rho}^1_R$, that $\langle \Delta \hat{S}_{x1}^2 \rangle_R \langle \Delta \hat{S}_{y1}^2 \rangle_R \geq \frac{1}{4} | \langle \hat{S}_{z1} \rangle_R |^2$, so for the conditioned variances associated with a separable state

$$\langle \Delta \hat{S}_{x1}^2 \rangle_{\tilde{S}_{x2}} \langle \Delta \hat{S}_{y1}^2 \rangle_{\tilde{S}_{y2}} \geq \frac{1}{4} \left( \sum_R P_R \left| \langle \hat{S}_{z1} \rangle_R \right| \right)^2$$

$$> \frac{1}{4} \left( \sum_R P_R \langle \hat{S}_{z1} \rangle_R \right)^2$$

$$= \frac{1}{4} \langle \hat{S}_{z1} \rangle^2$$  \hspace{1cm} (175)

showing that for a separable state the conditioned variances $\langle \Delta \hat{S}_{x1}^2 \rangle_{\tilde{S}_{x2}}$ and $\langle \Delta \hat{S}_{y1}^2 \rangle_{\tilde{S}_{y2}}$ still satisfy the HUP. It is important to note that these variances were associated with two different conditioned states based on two different measurements - spin $\hat{S}_{x2}$ and spin $\hat{S}_{y2}$ - carried out on sub-system 2, the results of which the observer for sub-system 1 would be unaware of. Thus if the EPR violations as defined in Eq.(159) are to occur then the state must be entangled.
Appendix G  Bell Inequality Proof

G.1 LHV Prediction

Here we set out the proof of the Bell inequalities following [18]. From the basic LHV result (43) for the mean value \( \langle A_i \times B_j \rangle_{LHV} \) we have

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

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

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

(176)

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

\[
|\langle A_2 \times B_1 \rangle_{LHV} - \langle A_2 \times B_2 \rangle_{LHV}| \\
\leq \int d\xi P(\xi) \langle |A_2(\xi)| \rangle \langle |B_1(\xi)| \rangle (1 \pm \langle A_1(\xi) \rangle ⟨ B_2(\xi) ⟩)
\]

\[
+ \int d\xi P(\xi) \langle |A_2(\xi)| \rangle \langle |B_2(\xi)| \rangle (1 \pm \langle A_1(\xi) \rangle ⟨ B_1(\xi) ⟩)
\]

(177)

where we have used the results that \( |\langle A_2(\xi) \rangle|, |\langle B_1(\xi) \rangle| \) and \( |\langle B_2(\xi) \rangle| \) are all less than unity and that \( \int d\xi P(\xi) = 1 \). Hence since \( |\langle A_1 \times B_2 \rangle_{LHV} + \langle A_1 \times B_1 \rangle_{LHV}| = +⟨\langle A_1 \times B_2 \rangle_{LHV} + \langle A_1 \times B_1 \rangle_{LHV}⟩ \) or \( -⟨\langle A_1 \times B_2 \rangle_{LHV} + \langle A_1 \times B_1 \rangle_{LHV}⟩ \) we have

\[
|\langle A_2 \times B_1 \rangle_{LHV} - \langle A_2 \times B_2 \rangle_{LHV}| \pm |\langle A_1 \times B_2 \rangle_{LHV} + \langle A_1 \times B_1 \rangle_{LHV}| \leq 2
\]

(178)

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

\[
|\langle A_2 \times B_1 \rangle_{LHV} - \langle A_2 \times B_2 \rangle_{LHV} + \langle A_1 \times B_1 \rangle_{LHV}| \leq 2
\]

(179)

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

G.2 Non-Entangled State Result

It can be shown that the Bell inequalities also always occur for non-entangled states (see Section 7.3 of the book by Vedral [17]). For Bell’s inequalities we consider Hermitian operators $\hat{A}_i$ and $\hat{B}_j$ for subsystems $A$, $B$ respectively, for which there are two eigenvalues $+1$ and $-1$, where examples of the operators are given by the components $\hat{A}_i = a_i \cdot \hat{\sigma}_A$ and $\hat{B}_j = b_j \cdot \hat{\sigma}_B$ of Pauli spin operators $\hat{\sigma}_A$ and $\hat{\sigma}_B$ along directions with unit vectors $a_i$ and $b_j$. The corresponding quantum theory quantity for the Bell inequality is

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

(180)

where in quantum theory the mean value is given by $E(\hat{A}_i \otimes \hat{B}_j) = \langle \hat{A}_i \otimes \hat{B}_j \rangle = Tr(\hat{\rho} \hat{A}_i \hat{B}_j)$. For the general bipartite non-entangled state given by 3 it is easy to show that

$$S = \sum_R P_R \left( \langle \hat{A}_1 \rangle_R^A \langle \hat{B}_1 + \hat{B}_2 \rangle_R^B + \langle \hat{A}_2 \rangle_R^A \langle \hat{B}_1 - \hat{B}_2 \rangle_R^B \right)$$

(181)

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

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

$$\leq 2$$

(182)

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

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Appendix H  Correlations and Entanglement

In this Appendix we derive a correlation inequality that applies for all separable states. Its violation would therefore be a sufficiency test for entanglement.

In quantum theory the correlation functions are given by $\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle = \text{Tr}(\hat{\rho} \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B)$ and $\langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle = \text{Tr}(\hat{\rho} \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B)$. For a non-entangled state of sub-systems $A$ and $B$ we have

$$\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle = \sum_R P_R \langle \hat{\Omega}_A^\dagger \rangle_R^A \langle \hat{\Omega}_B \rangle_R^B$$

$$\langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle = \sum_R P_R \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \rangle_R^A \langle \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle_R^B$$  \hspace{1cm} (183)

Now

$$|\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle| \leq \sum_R P_R |\langle \hat{\Omega}_A^\dagger \rangle_R^A| |\langle \hat{\Omega}_B \rangle_R^B|$$  \hspace{1cm} (184)

since the modulus of a sum is always less than the sum of the moduli. Using the inequality $\langle \hat{\Omega}_C^\dagger - \langle \hat{\Omega}_C \rangle \rangle \geq 0$ with $(C = A, B)$, we obtain the Cauchy-Schwarz inequality - which is true for all states - $\langle \hat{\Omega}_C^\dagger \hat{\Omega}_C \rangle \geq \langle \hat{\Omega}_C \rangle^2$, and hence

$$|\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle| \leq \sum_R P_R \sqrt{\langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \rangle_R^A} \sqrt{\langle \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle_R^B}$$  \hspace{1cm} (185)

Next we use the inequality

$$\sum_R P_R C_R \geq \left( \sum_R P_R \sqrt{C_R} \right)^2$$  \hspace{1cm} (186)

for real, positive functions $C_R, P_R$ and where $\sum_R P_R = 1$. This inequality, which was used in the paper by Hillery et al [61], is proved in Appendix E. In the present case we have $C_R = \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \rangle_R^A \langle \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle_R^B$ so that

$$|\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle|^2 \leq \sum_R P_R \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \rangle_R^A \langle \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle_R^B = \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle$$  \hspace{1cm} (187)

Thus for a non-entangled state we obtain the correlation inequality

$$|\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle|^2 = |\langle \hat{\Omega}_A \otimes \hat{\Omega}_B \rangle|^2 \leq \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle$$  \hspace{1cm} (188)

where the general result $\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle = (\hat{\Omega}_A \otimes \hat{\Omega}_B)^*$ has been used. Thus non-entangled states have correlation functions that are consistent with hidden variable theory, as would be expected since separable states are Bell local.
Appendix I  Extracting Entanglement due to Symmetrization

I.1 Two Particle Case - Bosons

The approach of Killoran et al [99] can be first applied to the simple case of \( N = 2 \) bosons initially in the \( A \) modes \( a0 \) and \( a1 \) and were discussed in SubSection 3.1.2. Here we present the detailed derivation of the results. The \( B \) modes \( b0 \) and \( b1 \) are initially unoccupied.

The occupied state is

\[
|\Phi_A \rangle = \frac{1}{\sqrt{2}} \left( |a0(1)\rangle |a1(2)\rangle + |a0(2)\rangle |a1(1)\rangle \right)
\]  

(189)

in first quantization. This is regarded by Killoran et al [99] as an entangled state for sub-systems consisting of particle 1 and particle 2. In second quantization the occupied state \( |\Phi_A \rangle \) and the unoccupied state \( |\Phi_B \rangle \) are given by

\[
|\Phi_A \rangle = |1\rangle_{a0} |1\rangle_{a1} \quad |\Phi_B \rangle = |0\rangle_{b0} |0\rangle_{b1}
\]

\[
|\Phi_A \rangle = \frac{1}{\sqrt{2}} \left( \hat{a}_0^\dagger \hat{a}_1^\dagger |0\rangle_{a0} |0\rangle_{a1} \right) + \frac{1}{\sqrt{2}} \left( \hat{a}_0^\dagger \hat{a}_1^\dagger |1\rangle_{b0} |1\rangle_{b1} \right)
\]

(190)

These are regarded as separable states for the \( A \) modes \( a0 \) and \( a1 \) and separable states for the \( B \) modes \( b0 \) and \( b1 \).

In second quantization we consider the effect of the beam splitter on an \( \text{input} \) state

\[
|\Phi_{in} \rangle = |\Phi_A \rangle \otimes |\Phi_B \rangle
\]

(191)

The effect is to produce an \( \text{output} \) state given by

\[
|\Phi_{out} \rangle = \tilde{U} |\Phi_{in} \rangle
\]

\[
= \frac{r_b \hat{b}_0^\dagger + t_b \hat{a}_0^\dagger}{\sqrt{T}} \frac{r_b \hat{b}_1^\dagger + t_b \hat{a}_1^\dagger}{\sqrt{T}} |0\rangle_{a0} |0\rangle_{a1} \otimes |0\rangle_{b0} |0\rangle_{b1}
\]

\[
+ \frac{r_b t_a}{\sqrt{T}} (|1\rangle_{a0} |1\rangle_{a1} \otimes |0\rangle_{b0} |0\rangle_{b1}) + rt (|0\rangle_{a0} |1\rangle_{a1} \otimes |1\rangle_{b0} |0\rangle_{b1})
\]

\[
+ r^2 (|0\rangle_{a0} |1\rangle_{a1} \otimes |1\rangle_{b0} |1\rangle_{b1}) + t^2 (|1\rangle_{a0} |0\rangle_{a1} \otimes |0\rangle_{b0} |1\rangle_{b1})
\]

(192)

Measurements can then be done on the output state based on projecting the state onto eigenstates for the number operators for the \( A \) and \( B \) mode-based sub-systems. The projectors \( \hat{\Pi}^A(N_A) \) for sub-system \( A \) onto eigenstates with \( N_A = 0, 1, 2 \) bosons are given by

\[
\hat{\Pi}^A(0) = |0\rangle_{a0} |0\rangle_{a1} \langle 0|_{a0} \langle 0|_{a1}
\]

\[
\hat{\Pi}^A(1) = |1\rangle_{a0} |0\rangle_{a1} \langle 1|_{a0} \langle 0|_{a1} + |0\rangle_{a0} |1\rangle_{a1} \langle 0|_{a0} \langle 1|_{a1}
\]

\[
\hat{\Pi}^A(2) = |2\rangle_{a0} |0\rangle_{a1} \langle 2|_{a0} \langle 0|_{a1} + |1\rangle_{a0} |1\rangle_{a1} \langle 1|_{a0} \langle 1|_{a1} + |0\rangle_{a0} |2\rangle_{a1} \langle 0|_{a0} \langle 2|_{a1}
\]

(193)
with corresponding expressions for projectors $\hat{\Pi}^B(N_B)$ for sub-system $B$.

To demonstrate entanglement extraction for particle based sub-systems with particle 1 in one sub-system, and particle 2 in the other sub-system we choose projectors corresponding to there being one particle in the $A$ modal sub-system and one particle being in the $B$ modal sub-system. Thus the output state is projected onto the states with $N_A = 1$ and $N_B = 1$ and we get after normalizing

$$|\Phi_{out}(1,1)\rangle = \frac{1}{\sqrt{2}}(|1\rangle_{a0} |0\rangle_{a1} \otimes |0\rangle_{b0} |1\rangle_{b1} + |0\rangle_{a0} |1\rangle_{a1} \otimes |1\rangle_{b0} |0\rangle_{b1})$$

(194)

This is still a bipartite entangled state of the of two modal sub-systems, $A$ and $B$.

If we construct a mathematical correspondence of the form

$$|a0(1)\rangle \rightarrow |1\rangle_{a0} |0\rangle_{a1} \quad |a1(2)\rangle \rightarrow |0\rangle_{b0} |1\rangle_{b1}$$

$$|a1(1)\rangle \rightarrow |0\rangle_{a0} |1\rangle_{a1} \quad |a0(2)\rangle \rightarrow |1\rangle_{b0} |0\rangle_{b1}$$

(195)

we see that the projected output state given in (194) as a bipartite entangled state of the of two modal sub-systems, $A$ and $B$, has the same mathematical form as the bipartite entangled state of the of two particle sub-systems containing particle 1 and particle 2, respectively.

### I.2 Two Particle Case - Fermions

Here the details for the simple case of $N = 2$ fermions initially in the $C$ modes $c0$ and $c1$ are presented, following the same approach as in the previous SubSection. The $D$ modes $d0$ and $d1$ are initially unoccupied. Fermion modes are denoted $c$ and $d$ to distinguish them from bosonic modes $a$ and $b$.

The occupied state is

$$|\Phi_C\rangle = \frac{1}{\sqrt{2}}\{|c0(1)\rangle |c1(2)\rangle - |c0(2)\rangle |c1(1)\rangle\}$$

(196)

in first quantization. This is regarded by Killoran et al [99] as an entangled state for sub-systems consisting of particle 1 and particle 2. In second quantization the occupied state $|\Phi_C\rangle$ and the unoccupied state $|\Phi_D\rangle$ are given by

$$|\Phi_C\rangle = |1\rangle_{c0} |1\rangle_{c1} \quad |\Phi_D\rangle = |0\rangle_{d0} |0\rangle_{d1}$$

$$|\Phi_C\rangle = \frac{(c^0_0)}{\sqrt{1}} |0\rangle_{c0} |0\rangle_{c1} \quad |\Phi_D\rangle = |0\rangle_{d0} |0\rangle_{d1}$$

(197)

These are regarded as separable states for the $C$ modes $c0$ and $c1$ and separable states for the $D$ modes $d0$ and $d1$. 
In second quantization we consider the effect of the beam splitter on an input state

$$|\Phi_{in}\rangle = |\Phi_C\rangle \otimes |\Phi_D\rangle$$

(198)

The effect is to produce an output state given by

$$|\Phi_{out}\rangle = \hat{U} |\Phi_{in}\rangle$$

$$= \frac{(r \hat{a}_0^\dagger + t \hat{c}_1^\dagger)}{\sqrt{1}} (r \hat{a}_0^\dagger + t \hat{c}_1^\dagger) |0\rangle_{c0} |0\rangle_{c1} \otimes |0\rangle_{d0} |0\rangle_{d1}$$

$$= r^2 (|0\rangle_{c0} |0\rangle_{c1} \otimes |1\rangle_{d0} |1\rangle_{d1}) + rt(- |0\rangle_{c0} |1\rangle_{c1} \otimes |1\rangle_{d0} |0\rangle_{d1} + |1\rangle_{c0} |0\rangle_{c1} \otimes |0\rangle_{d0} |1\rangle_{d1})$$

$$+ t^2 (|1\rangle_{c0} |1\rangle_{c1} \otimes |0\rangle_{d0} |0\rangle_{d1})$$

(199)

Note the minus sign in the second term - this is due to the fermion creation and one particle being in the $D$ and $N$ projected onto the states with corresponding expressions for projectors $\hat{\Pi}_C(N_C)$ for sub-system $C$ onto eigenstates with $N_C = 0, 1, 2$ bosons are given by

$$\hat{\Pi}^C(0) = |0\rangle_{c0} |0\rangle_{c1} \langle 0|_{c0} \langle 0|_{c1}$$

$$\hat{\Pi}^C(1) = (|1\rangle_{c0} |0\rangle_{c1} \langle 1|_{c0} \langle 0|_{c1} + |0\rangle_{c0} |1\rangle_{c1} \langle 0|_{c0} \langle 1|_{c1})$$

$$\hat{\Pi}^C(2) = (|2\rangle_{c0} |0\rangle_{c1} \langle 2|_{c0} \langle 0|_{c1} + |1\rangle_{c0} |1\rangle_{c1} \langle 1|_{c0} \langle 1|_{c1} + |0\rangle_{c0} |2\rangle_{c1} \langle 0|_{c0} \langle 2|_{c1})$$

(200)

with corresponding expressions for projectors $\hat{\Pi}^D(N_D)$ for sub-system $D$. To demonstrate entanglement extraction for particle based sub-systems with particle 1 in one sub-system, and particle 2 in the other sub-system we choose projectors corresponding to there being one particle in the $C$ modal sub-system and one particle being in the $D$ modal sub-system. Thus the output state is projected onto the states with $N_C = 1$ and $N_D = 1$ and we get after normalizing

$$|\Phi_{out}(1,1)\rangle = \mathcal{N} (\hat{\Pi}^C(1) \otimes \hat{\Pi}^D(1)) |\Phi_{out}\rangle$$

$$= \frac{1}{\sqrt{2}} (|1\rangle_{c0} |0\rangle_{c1} \otimes |0\rangle_{d0} |1\rangle_{d1} - |0\rangle_{c0} |1\rangle_{c1} \otimes |1\rangle_{d0} |0\rangle_{d1})$$

(201)

This is still a bipartite entangled state of the of two modal sub-systems, $C$ and $D$. If we construct a mathematical correspondence of the form

$$|c0(1)\rangle \rightarrow |1\rangle_{c0} |0\rangle_{c1} \quad |c1(2)\rangle \rightarrow |0\rangle_{d0} |1\rangle_{d1}$$

$$|c1(1)\rangle \rightarrow |0\rangle_{c0} |1\rangle_{c1} \quad |c0(2)\rangle \rightarrow |1\rangle_{d0} |0\rangle_{d1}$$

(202)

we see that the projected output state given in (201) as a bipartite entangled state of the of two modal sub-systems, $C$ and $D$, has the same mathematical form as the bipartite entangled state of the of two particle sub-systems containing particle 1 and particle 2, respectively - even down to the correct minus sign in the second term.
I.3 Three Particle Case - Bosons

The key ideas in the approach by Killoran et al [99] are more fully illustrated by considering one of their specific cases, namely a quantum state with \( N = 3 \) identical bosons for a system with four modes - two \( A \) modes \( a_0 \) and \( a_1 \) and two \( B \) modes \( b_0 \) and \( b_1 \) - in which there are two bosons in mode \( a_0 \) and one boson in mode \( a_1 \). The other modes \( b_0 \) and \( b_1 \) are initially unoccupied. The modes \( a_0 \) and \( b_0 \) could be two different spatial modes for a bosonic atom in one hyperfine state, and \( a_1 \) and \( b_1 \) could be two different spatial modes for a bosonic atom in another hyperfine state. With particles labelled 1, 2 and 3 the quantum state in terms of first quantization is given by

\[
|\Phi_A\rangle = \frac{1}{\sqrt{12}} \left( |a_0(1)\rangle |a_0(2)\rangle |a_1(3)\rangle + |a_0(1)\rangle |a_0(3)\rangle |a_1(2)\rangle + |a_0(2)\rangle |a_0(1)\rangle |a_1(3)\rangle + |a_0(2)\rangle |a_0(3)\rangle |a_1(1)\rangle + |a_0(3)\rangle |a_0(1)\rangle |a_1(2)\rangle + |a_0(3)\rangle |a_0(2)\rangle |a_1(1)\rangle \right)
\]

(203)

In first quantization there is no state for the \( B \) modes, since the vacuum state is not recognized as a quantum state of anything. Following the approach of regarding labelled identical particles as sub-systems we consider a bipartite division of the three particle system with the first sub-system as consisting of particle 1 and 2 and the second sub-system consisting of particle 3. The same state \( |\Phi_A\rangle \) can be written as

\[
|\Phi_A\rangle = \frac{1}{\sqrt{3}} \left( |a_0(1)\rangle |a_0(2)\rangle |a_1(3)\rangle + \frac{\sqrt{2}}{3} \left( |a_0(1)\rangle |a_1(2)\rangle + |a_0(2)\rangle |a_1(1)\rangle \right) |a_0(3)\rangle \right)
\]

(204)

In this form the state appears to be an entangled state for the two sub-systems. The first term (which has amplitude \( 1/\sqrt{3} \)) represents a state for the sub-system of particle 1 and 2 with both particles in single particle state \( |a_0\rangle \) and a state for the sub-system of particle 3 with particles in single particle state \( |a_1\rangle \). The second term (which has amplitude \( \sqrt{2}/3 \)) represents a state for the sub-system of particles 1 and 2 with one particles in single particle state \( |a_0\rangle \) and the other in single particle state \( |a_1\rangle \), and a state for the sub-system of particle 3 with this particle in single particle state \( |a_0\rangle \). It is this entanglement which Killoran et al [99] wish to extract by applying a beam splitter to the state \( |\Phi_A\rangle \), the beam splitter being associated with a unitary operator \( \hat{U} \) whose effect is to transform the single particle states \( |ak\rangle \) and \( |bk\rangle \) into linear combinations of each other involving reflection and transmission coefficients \( r, t \) as follows

\[
\hat{U} |ak\rangle = r |bk\rangle + t |ak\rangle \quad k = 0, 1
\]

\[
\hat{U} |bk\rangle = t |bk\rangle - r |ak\rangle \quad k = 0, 1
\]

(205)

For simplicity \( r, t \) are assumed to be real with \( r^2 + t^2 = 1 \). The beam splitter is just assumed to couple spatial modes of the same hyperfine state. This unitary...
operator applies irrespective of the particular particle occupying the one particle states.

In second quantization the occupied state $|\Phi_A\rangle$ and the unoccupied state $|\Phi_B\rangle$ are given by

$$
|\Phi_A\rangle = |2\rangle_{a0} |1\rangle_{a1} \quad |\Phi_B\rangle = |0\rangle_{b0} |0\rangle_{b1}
$$

$$
|\Phi_A\rangle = \left(\frac{\hat{a}_b^\dagger}{\sqrt{2}} \frac{\hat{a}_a^\dagger}{\sqrt{1}}\right) |0\rangle_{a0} |0\rangle_{a1} \quad |\Phi_B\rangle = |0\rangle_{b0} |0\rangle_{b1} \quad (206)
$$

where the Fock states are also written in terms of mode creation operators and vacuum states for the modes. In second quantization it is clear that the Fock states are also written in terms of mode creation operators and vacuum states for the modes. In second quantization it is clear that $|\Phi_A\rangle$ and $|\Phi_B\rangle$ themselves are respectively separable states for the $A$ and $B$ modes. In second quantization the effect of the unitary operator associated with the beam splitter follows from (205) noting that $|ak\rangle \equiv \hat{a}_k^\dagger |0\rangle$ and $|bk\rangle \equiv \hat{b}_k^\dagger |0\rangle$ and is given by

$$
\hat{U} \hat{a}_k^\dagger \hat{U}^{-1} = r\hat{b}_k^\dagger + t \hat{a}_k^\dagger \quad \hat{U} \hat{b}_k^\dagger \hat{U}^{-1} = \hat{b}_k^\dagger - r \hat{a}_k^\dagger \quad k = 0, 1 \quad (207)
$$

In paper II we show that two mode beam splitters can indeed be described by equations analogous to (207). In second quantization we consider the effect of the beam splitter on an input state

$$
|\Phi_{in}\rangle = |\Phi_A\rangle \otimes |\Phi_B\rangle \quad (208)
$$

The effect is to produce an output state given by

$$
|\Phi_{out}\rangle = \hat{U} |\Phi_{in}\rangle = \frac{(r\hat{b}_0^\dagger + t\hat{a}_0^\dagger)^2 (r\hat{b}_1^\dagger + t\hat{a}_1^\dagger)}{\sqrt{2}} |0\rangle_{a0} |0\rangle_{a1} \otimes |0\rangle_{b0} |0\rangle_{b1}
$$

$$
= r^3 |0\rangle_{a0} |0\rangle_{a1} \otimes |2\rangle_{b0} |1\rangle_{b1} + r^2 t (|0\rangle_{a0} |1\rangle_{a1} \otimes |2\rangle_{b0} |0\rangle_{b1} + \sqrt{2} (|1\rangle_{a0} |0\rangle_{a1} \otimes |1\rangle_{b0} |1\rangle_{b1})
$$

$$
+ r t^2 (|2\rangle_{a0} |0\rangle_{a1} \otimes |0\rangle_{b0} |1\rangle_{b1} + \sqrt{2} (|1\rangle_{a0} |1\rangle_{a1} \otimes |1\rangle_{b0} |0\rangle_{b1}) + t^3 (|2\rangle_{a0} |1\rangle_{a1} \otimes |0\rangle_{b0} |0\rangle_{b1}) \quad (209)
$$

Note this state is normalized to unity as $\langle \Phi_{out} | \Phi_{out} \rangle = (r^2 + t^2)^3 = 1$. The input state is a bipartite separable state of two modal sub-systems, one containing the two $A$ modes $a0$ and $a1$ and the other the two $B$ modes $b0$ and $b1$. The output state terms each are eigenstates of number operators $\hat{N}_A = \hat{a}_0^\dagger \hat{a}_0 + \hat{a}_1^\dagger \hat{a}_1$ and $\hat{N}_B = \hat{b}_0^\dagger \hat{b}_0 + \hat{b}_1^\dagger \hat{b}_1$ with eigenvalues $N_A = 0$, $N_B = 3$ for the $r^3$ term, $N_A = 1$, $N_B = 2$ for the $r^2 t$ term, $N_A = 2$, $N_B = 1$ for the $r t^2$ term, $N_A = 3$, $N_B = 0$ for the $t^3$ term. The same result as in (209) can also be obtained using (205) in conjunction with the first quantization form of the input state given by (203) though the algebra is more complex. In contrast to the input state, the output state is a bipartite entangled state of two modal sub-systems, one containing the two $A$ modes $a0$ and $a1$ and the other the two $B$ modes $b0$ and $b1$. Both input and output states are states with the same total of $N = 3$ bosons.

S 30
Measurements can then be done on the output state based on projecting the state onto eigenstates for the number operators for the A and B mode-based sub-systems. The projectors $\hat{\Pi}^A(N_A)$ for sub-system A onto eigenstates with $N_A = 0, 1, 2, 3$ bosons are given by

$$\hat{\Pi}^A(0) = \langle 0 \rangle_{a0} \langle 0 \rangle_{a1} \langle 0 \rangle_{a0} \langle 0 \rangle_{a1}$$

$$\hat{\Pi}^A(1) = \langle 1 \rangle_{a0} \langle 0 \rangle_{a1} \langle 1 \rangle_{a0} \langle 0 \rangle_{a1} + \langle 0 \rangle_{a0} \langle 1 \rangle_{a0} \langle 0 \rangle_{a1} \langle 1 \rangle_{a1} + \langle 0 \rangle_{a0} \langle 0 \rangle_{a1} \langle 1 \rangle_{a0} \langle 1 \rangle_{a1}$$

$$\hat{\Pi}^A(2) = \langle 2 \rangle_{a0} \langle 0 \rangle_{a1} \langle 2 \rangle_{a0} \langle 0 \rangle_{a1} + \langle 1 \rangle_{a0} \langle 1 \rangle_{a0} \langle 0 \rangle_{a1} \langle 1 \rangle_{a1} + \langle 0 \rangle_{a0} \langle 1 \rangle_{a0} \langle 0 \rangle_{a1} \langle 2 \rangle_{a1} + \langle 0 \rangle_{a0} \langle 2 \rangle_{a1} \langle 0 \rangle_{a0} \langle 0 \rangle_{a1}$$

$$\hat{\Pi}^A(3) = \langle 3 \rangle_{a0} \langle 0 \rangle_{a1} \langle 3 \rangle_{a0} \langle 0 \rangle_{a1} + \langle 2 \rangle_{a0} \langle 1 \rangle_{a0} \langle 0 \rangle_{a1} \langle 1 \rangle_{a1} + \langle 1 \rangle_{a0} \langle 2 \rangle_{a0} \langle 1 \rangle_{a0} \langle 0 \rangle_{a1} + \langle 0 \rangle_{a0} \langle 3 \rangle_{a1} \langle 0 \rangle_{a0} \langle 0 \rangle_{a1}$$

with corresponding expressions for projectors $\hat{\Pi}^B(N_B)$ for sub-system B.

To demonstrate entanglement extraction for particle based sub-systems with particles 1 and 2 in one sub-system, and particle 3 in the other sub-system we choose projectors corresponding to there being two particles in the $A$ modal sub-system and one particle being on the $B$ modal sub-system. Thus the output state is projected onto the states with $N_A = 2$ and $N_B = 1$ and we get after normalizing

$$|\Phi_{\text{out}}(2, 1)\rangle = \mathcal{N} \left( \hat{\Pi}^A(2) \otimes \hat{\Pi}^B(1) \right) |\Phi_{\text{out}}\rangle$$

$$= \frac{1}{\sqrt{3}} \langle 2 \rangle_{a0} \langle 0 \rangle_{a1} \otimes \langle 0 \rangle_{b0} \langle 1 \rangle_{b1} + \sqrt{\frac{2}{3}} \langle 0 \rangle_{a0} \langle 1 \rangle_{a0} \langle 0 \rangle_{b0} \langle 1 \rangle_{b1}$$

(211)

This is still a bipartite entangled state of the of two modal sub-systems, $A$ and $B$.

If we construct a mathematical correspondence of the form

$$|a0(1)\rangle \langle a0(2)| \rightarrow |2\rangle_{a0} \langle 0 \rangle_{a1} \quad |a1(3)\rangle \rightarrow |0\rangle_{a0} \langle 1 \rangle_{b1}$$

$$\frac{1}{\sqrt{2}} \{|a0(1)\rangle \langle a1(2)| + |a0(2)\rangle \langle a1(1)|\rangle \rightarrow |1\rangle_{a0} \langle 1 \rangle_{a1} \quad |a0(3)\rangle \rightarrow |1\rangle_{a0} \langle 0 \rangle_{b1}$$

(212)

we see that the projected output state given in (211) as a bipartite entangled state of the of two modal sub-systems, $A$ and $B$, has the same mathematical form as the bipartite entangled state of the of two particle sub-systems containing particles 1 and 2 and particle 3, respectively. This type of result is proved in more general cases in [99] - here we have exhibited the key features of their approach in a particular case.

It is on this basis that Killoran et al [99] assert that the action of the beam splitter is to extract the entanglement due to symmetrization that was present in the quantum state $|\Phi_A\rangle$ for the particle sub-systems containing particles 1 and 2 and particle 3, respectively. It is of course not their ingenious mathematical derivation that is in dispute - it is the interpretation. From the point of view
of sub-systems being modes, not particles the action of the beam splitter is to create an entangled state of the two modal sub-systems, $A$ and $B$ from a state that was separable. That this entangled output state can be projected onto eigenstates of the number operators for the two modal sub-systems, $A$ and $B$ which have the same mathematical form as the presumed entangled initial state for the particle sub-systems containing particles 1 and 2 and particle 3, respectively is of course interesting, but it does not show that labeled identical particles can be regarded as physically accessible sub-systems. Apart from the logical issue that sub-systems must be both distinguishable from each other via physical measurements, it is noteworthy that the approach of Killoran et al [99] rested on physical processes that involved coupling modes, not identified indistinguishable particles.
Appendix J  

Proof of Quantum Correlation Results

In this Appendix we prove a theorem and its corollaries regarding quantum correlation functions for global SSR compliant states (see Section 3.2.6).

J.1 Theorem Proof

If the state is global particle number SSR compliant then if we choose a complete orthonormal set of Fock states $|N, \alpha\rangle$ with $\alpha = 1, 2, \ldots, d_N$ listing states which are eigenstates of the total number operator $\hat{N}$ with eigenvalue $N$ we can write the density operator in the form

$$\hat{\rho} = \sum_{N} \sum_{\alpha,\beta} P_{N,\alpha,\beta}^N |N, \alpha\rangle \langle N, \beta|$$ (213)

where since $\text{Tr} \hat{\rho} = 1$ we must have

$$1 = \sum_{N} \sum_{\alpha} P_{N,\alpha,\alpha}^N$$ (214)

Now $(\hat{a}^\dagger)^n (\hat{a})^m (\hat{b}^\dagger)^l (\hat{b})^k |N, \alpha\rangle$ must be a linear combination of Fock states with $N$ replaced by $N + n + l - m - k$ so we can write

$$(\hat{a}^\dagger)^n (\hat{a})^m (\hat{b}^\dagger)^l (\hat{b})^k |N, \alpha\rangle = \sum_{\gamma} C_{N,\alpha,\gamma}^N (n, m, l, k) |(N + n + l - m - k), \gamma\rangle$$ (215)

Hence

$$\langle (\hat{a}^\dagger)^n (\hat{a})^m (\hat{b}^\dagger)^l (\hat{b})^k \rangle = \text{Tr} \left( \sum_{N} \sum_{\alpha,\beta} P_{N,\alpha,\beta}^N \sum_{\gamma} C_{N,\alpha,\gamma}^N (n, m, l, k) |(N + n + l - m - k), \gamma\rangle \langle N, \beta| \right)$$ (216)

But $\text{Tr} |(N + n + l - m - k), \gamma\rangle \langle N, \beta| = 0$ unless $n + l - m - k = 0$. Hence

$$\langle (\hat{a}^\dagger)^n (\hat{a})^m (\hat{b}^\dagger)^l (\hat{b})^k \rangle = 0 \text{ if } n + l \neq m + k$$ (217)

which is the required theorem.

J.2 Corollaries Proof

The first corollary follows immediately from the theorem.

To prove the second corollary we consider a state which is non globally SSR compliant. If the state is non-compliant then its density operator must contain a contribution which allows for non-zero coherences between Fock states with different $N$. We can therefore write the density operator as

$$\hat{\rho} = \sum_{N} \sum_{\alpha,\beta} P_{N,\alpha,\beta}^N |N, \alpha\rangle \langle N, \beta| + \sum_{N \neq M} \sum_{\alpha,\beta} P_{N,\alpha,\beta}^{N,M} |N, \alpha\rangle \langle M, \beta|$$ (218)
where the second term is the **SSR non-compliant contribution**.

A similar calculation to before for the situation when \( n + l = m + k \) gives

\[
\langle (\hat{a}^\dagger)^n (\hat{a})^m (\hat{b}^\dagger)^l (\hat{b})^k \rangle = \text{Tr}\left( \sum_N \sum_{\alpha,\beta} P_N^{N} \sum_{\gamma} C_N^{N}(n, m, l, k) |N, \gamma\rangle \langle N, \beta| \right)
\]

\[
+ \text{Tr}\left( \sum_{N \neq M} \sum_{\alpha,\beta} P_N^{N} \sum_{\gamma} C_N^{N}(n, m, l, k) |N, \gamma\rangle \langle M, \beta| \right)
\]

(219)

But \( \text{Tr}(|N, \gamma\rangle \langle M, \beta|) = 0 \) for \( N \neq M \), so the non-compliant contribution gives zero and as \( \text{Tr}(|N, \gamma\rangle \langle N, \beta|) = \delta_{\gamma, \beta} \) we end up with

\[
\langle (\hat{a}^\dagger)^n (\hat{a})^m (\hat{b}^\dagger)^l (\hat{b})^k \rangle = \left( \sum_N \sum_{\alpha,\beta} P_N^{N} C_N^{N}(n, m, l, k) \right)
\]

(220)

which is entirely dependent on the contribution to the density operator that is globally SSR compliant. Measurements of this type with \( n + l = m + k \) would therefore not respond to the presence of contribution to the density operator that is not globally SSR compliant. The BS measurements discussed in paper II are all of this type, so will not test the super-selection rule.
Appendix K  Reference Frames and Super-Selection Rules

Several papers such as [69], [71], [60], [63], [40], [64], [65] explain the link between reference frames and super-selection rules (SSR). In this Appendix we present the key ideas involved.

K.1 Two Observers with Different Reference Frames

The first point to appreciate is that there are two observers - Alice and Charlie - who are involved in describing the same quantum system, which has been prepared via some physical process. We will refer to Charlie as the external observer, Alice the internal observer. The system could be a multi-mode system involving identical particles, it could just be a single mode system or it could even be a single particle with or without spin. Alice and Charlie each describe quantum states in terms of their own reference frames, which might be a set of coordinate axes for the case of the spin or position states for the single particle system, or it could be a large quantum system with a well-defined reference phase in the case of multi-mode or single mode systems involving identical particles.

Alice and Charlie may each choose from a set of possible reference frames - for the single particle case there are an infinite number of different choices of coordinate axes for example, related to each other via rotations and/or translations. In Situation A - which is not associated with SSR - Alice and Charlie do know the relationship between their two reference frames (and can communicate this relationship via classical communications) - such as in the case of the single particle system when the relative orientation of their two different coordinate axes are known. In Situation B - which is associated with SSR - Alice and Charlie do not know the relationship between their two reference frames - such as in the multi-mode or single mode system involving identical particles when the relative phase between their two large quantum phase reference systems is not known. Alice and Charlie describe the same system via density operators $\hat{\sigma}$ and $\hat{\rho}$, and the key question is the relationship between these two operators in situations A and B and for various types of reference frames. In terms of the notation in [60] $\rho \rightarrow \hat{\sigma}$ and $\hat{\rho} \rightarrow \hat{\rho}$. In some situations the assumption that Alice even possesses a well-defined reference frame may be invalid, in which case it is important to realize that it is Charlie’s quantum state which is of most interest for describing the system. This description may differ from what hypothetical observer Alice would regard as the quantum state.

K.2 Symmetry Groups

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

A few examples are as follows:

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

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

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

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

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

**K.3 Relationships - Situation A**

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

$$\hat{\rho} = \hat{T}(g) \hat{\sigma} \hat{T}(g)^{-1} \quad (221)$$
Note that this is a *passive* transformation - no change of state is involved, just the same state being described by two different observers.

As an example, consider the spinless particle and the translation group. If $|\hat{x}_a\rangle$ is a position eigenstate then $\hat{T}(a) |\hat{x}_a\rangle = |\hat{x}_a - a\rangle$. A pure quantum position eigenstate described by Alice as $|\hat{x}_a\rangle$ would be described by Charlie as $|\hat{x}_a - a\rangle$. This is as expected since Alice’s Cartesian axes have been translated by $a$ which is also a pure quantum position eigenstate but with eigenvalue $\hat{x}_a - a$. This is as expected since Alice’s Cartesian axes have been translated by $a$ to the origin of Charlie’s axes without change of orientation. In the case of momentum eigenstates $|\hat{p}_a\rangle$ we have $\hat{T}(a) |\hat{p}_a\rangle = \exp(ia \cdot a/\hbar) |\hat{p}_a\rangle$, so a pure quantum momentum eigenstate described by Alice with $|\hat{p}_a\rangle$ would be described by Charlie with $|\Psi\rangle = \exp(ia \cdot a/\hbar) |\hat{p}_a\rangle$, which is also a pure momentum eigenstate with the same eigenvalue $\hat{p}_a$. Alice and Charlie describe the pure momentum eigenstate with the same density operator $\hat{\rho} = \hat{\sigma}$, the phase factor cancels.

For more general pure states, consider a quantum state described by Alice as $|\Phi\rangle$ with state vector $|\Phi\rangle = \int d\hat{x}_a \hat{\Phi}(\hat{x}_a) |\hat{x}_a\rangle$. States of this form can represent *localized* states when $\hat{\Phi}(\hat{x}_a)$ is only significant in confined spatial regions, or they can represent *delocalized* states, such as momentum eigenstates $|\hat{p}_a\rangle$ when $\hat{\Phi}(\hat{x}_a) = (2\pi\hbar)^{-3/2} \exp(i \hat{p} \cdot \hat{x}_a/\hbar)$. We see that Charlie also describes a pure quantum state $|\Psi\rangle = \int d\hat{x}_a \hat{\Psi}(\hat{x}_a) |\hat{x}_a\rangle$, so the wavefunction is now $\hat{\Psi}(\hat{x}_a) = \hat{\Phi}(\hat{x}_a + a)$. Note that if Alice’s state vector was written in terms of momentum eigenstates $|\Phi\rangle = \int d\hat{p}_a \hat{\Phi}(\hat{p}_a) |\hat{p}_a\rangle$, then Charlie’s state vector $|\Psi\rangle = \int d\hat{p}_a \hat{\Psi}(\hat{p}_a) |\hat{p}_a\rangle$ has a momentum wave function $\hat{\Psi}(\hat{p}_a) = \exp(i \hat{p} \cdot a/\hbar) \hat{\Phi}(\hat{p}_a)$ related to that of Alice by a phase factor. Note that a state which is a quantum superposition of momentum eigenstates as described by Alice is also described as a quantum superposition of momentum eigenstates by Charlie. A similar feature applies in all situation A cases, and is related to SSR not applying in situation A.

The case of the *particle* with *spin* and the *rotation* group is outlined in Ref. [71].

### K.4 Relationships - Situation B

In *Situation B*, where on the other hand the relationship between frames is completely *unknown*, all possible transformations $g$ must be given *equal weight*, and hence the relationship between Alice’s and Charlie’s description of the same
state becomes

\[ \hat{\rho} = \int w(g)dg \hat{T}(g) \hat{\sigma} \hat{T}^{-1}(g) \]

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

It is straightforward to show that for any fixed parameter \( h \) that

\[ \hat{T}(h) \hat{\rho} \hat{T}^{-1}(h) = \hat{\rho} \]

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

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

It is straightforward to show that

\[ \hat{T}(\theta_a) |\Phi(\beta)\rangle = |\Phi(\beta \exp(i\theta_a))\rangle \]

so that the Glauber coherent state is transformed into another Glauber coherent state, but with \( \beta \) changed via a phase factor to \( \beta \exp(i\theta_a) \). The quantum state described by Charlie is given by

\[ \hat{\rho} = \int \frac{d\theta_a}{2\pi} |\Phi(\beta \exp(i\theta_a))\rangle \langle \Phi(\beta \exp(i\theta_a))| \]

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

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

\[ = \sum_{n_a} |C(n_a, \beta)|^2 |n_a\rangle \langle n_a| \]

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

which is a mixed state consisting of a Poisson distribution of Fock states with mean occupation number \( \bar{n}_a = |\beta|^2 \). In view of the first expression for \( \hat{\rho} \) it can also be thought of as a mixed state consisting of Glauber coherent states each with the same amplitude \( |\beta| = \sqrt{\bar{n}_a} \), but with all phases \( \arg(\beta + \theta_a) \) equally probable. Thus, whereas Alice describes the state as a pure state that
is a quantum superposition of Fock states with differing occupancy numbers, Charlie describes the same state as a mixed state involving a statistical mixture of number states. The former violates the SSR whereas the latter does not. A similar feature applies in all situation B cases, and is related to SSR applying in Situation B. Whether Alice could ever prepare such a state in the first place is controversial - see the discussion presented above in SubSections 3.2 and 3.4. However, assuming she could, the quantum state as described by Charlie is a mixed state.

The situation just studied relates of course to the debate [113] regarding whether the quantum state for a single mode laser operating well above threshold should be described by a Glauber coherent state or as a Poisson statistical mixture of photon number states. The first viewpoint (Alice) describes the state from the point of view of an internal observer with a reference frame, the second (Charlie) describes the same state from the point of view of an external observer for whose reference frame relationship to that of the internal observer is unknown. The debate is regarded by [71] as settled on the basis that both viewpoints are valid, they are just at cross purposes because they refer to descriptions of the same quantum state by two different observers.

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

K.5 Dynamical and Measurement Considerations

Discussions of the relationship between equations governing the dynamical behavior of Alice’s and Charlie’s density operators depend on whether the evolution is just governed by a Hamiltonian or whether master equations describing evolution affected by interactions with an external environment are involved. Such matters will not be treated in detail here, nor will the issue of relating
Alice’s and Charlie’s measurements. The latter issue is dealt with in [60].

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

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

(227)

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

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

(228)

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

K.6 Nature of Reference Frames

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

In this SubSection we will describe possible phase reference frames as if they are entirely separated (or uncorrelated) with the system of interest. In terms of the treatment by Bartlett et al [71], [60] these are non-implicated reference frames. In the next SubSection and in the next Appendix phase reference frames that are correlated with the system of interest will be described - these are the so-called implicated reference frames of Bartlett et al.

For the large quantum system with a well-defined reference phase associated with the \( U(1) \) group in the case of multi-mode or single mode systems involving identical particles, the usual choice is a single mode bosonic system such as a single mode BEC or a laser with a large mean occupancy, and which is thought of as being prepared in a Glauber coherent state \( |\Phi(\alpha)\rangle \) in order to provide the phase reference frame, the reference phase being \( \text{arg} \alpha \). Whether such a reference frame really exists is controversial. The discussion presented above in SubSections 3.2 and 3.4 raises the question of whether such a phase reference state could ever be prepared, so this choice of a physical phase reference is rather
unsatisfactory. However, from the point of view of this presentation we assume it does, so that - as in the previous example - Alice can describe the reference state as another coherent state. Again, whether Alice could ever prepare such a state is questionable.

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

$$|\theta_p\rangle = \frac{1}{\sqrt{n_{\text{max}} + 1}} \sum_{n=0}^{n_{\text{max}}} \exp(in\theta_p) |n\rangle$$  \hspace{1cm} (229)$$

These states are orthonormal. The separation between the equally spaced phase angles $\Delta\theta = 2\pi/(n_{\text{max}} + 1)$ can be made very small if $n_{\text{max}}$ is large enough. Under the effect of the harmonic oscillator Hamiltonian $\hat{H} = \hbar\omega \hat{N}$, where $\hat{N}$ is the number operator, the phase state $|\theta_p\rangle$ evolves into $|\theta_p - \omega\Delta t\rangle$ during a time interval $\Delta t$, so if the time intervals are chosen so that $\omega\Delta t = 2\pi/(n_{\text{max}} + 1)$, the phase angle $\theta_p$ changes into $\theta_p - 1$. Thus the system behaves like a backwards running clock [111], the phase angles $\theta_p$ defining the positions of the hands. If the clock initially has phase $\theta_p$ the probability of finding the clock to have phase $\theta_q$ after a time interval $\Delta t$ is given by

$$P(\theta_q, \theta_p, \Delta t) = \frac{1}{(n_{\text{max}} + 1)^2} \frac{\sin^2((n_{\text{max}} + 1)\Delta/2)}{\sin^2(\Delta/2)}$$  \hspace{1cm} (230)$$

where $\Delta = \theta_p - \theta_q - \omega\Delta t$. For times $\Delta t$ such that $\omega\Delta t \ll 2\pi/(n_{\text{max}} + 1)$ the probability of the phase remaining as $\theta_p$ is close to unity. Thus if the phase state $|\theta_p\rangle$ is used as a phase reference, it will remain stable for a time $\Delta t$ satisfying the last inequality. For $\Delta t \sim 100\mu s$ and $n_{\text{max}} \sim 10^4$ so that phase is defined to $\sim 10^{-3}$ radians, an oscillator frequency $\omega \sim 10^9 \text{ s}^{-1}$ would suffice for this phase reference standard. Such macroscopic oscillators do exist, though the process to prepare them in the phase reference quantum state $|\theta_p\rangle$ would be technically difficult. Whether such a system would be useful as a phase reference for optical fields or a BEC is another issue.

K.7 Relational Description of Phase References

In this SubSection phase reference frames that are correlated with the system of interest will be described - these are the so-called implicated reference frames of Bartlett et al [71], [60].

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

In the so-called internalization or quantization of the reference frame the product state \( |m\rangle_S \otimes |n\rangle_R \) is mapped onto the product state \( |m\rangle_S \otimes |n - m\rangle_R \) where \( n \geq m_{\text{max}} \). Thus

\[
|m\rangle_S \otimes |n\rangle_R \rightarrow |m\rangle_S \otimes |n - m\rangle_R
\]

Hence for a linear combination of system states given by

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

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

\[
|\Phi\rangle_S \otimes |n\rangle_R = \sum_{m=0}^{m_{\text{max}}} C_m |m\rangle_S \otimes |n\rangle_R \rightarrow \sum_{m=0}^{m_{\text{max}}} C_m |m\rangle_S \otimes |n - m\rangle_R = |\Psi_n\rangle_{RS}
\]

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

\[
\hat{\rho}_S = Tr_R(|\Psi_n\rangle_{RS} \langle \Psi|_{RS})
\]

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

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

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

\[
|m\rangle_S \otimes |n\rangle_R \rightarrow |m\rangle_S \otimes |m + n\rangle_R
\]
The mapping of the $H_S \otimes H_R$ state $|\Psi_n\rangle_{RS}$ then is

$$
|\Psi_n\rangle_{RS} = \sum_{m=0}^{m_{\text{max}}} C_m |m\rangle_S \otimes |n-m\rangle_R
$$

The mapping results in a non-entangled state which is incompatible with the SSR. The state in the subspace $H_S$ is a coherent superposition of number states, whilst that in $H_R$ is a Fock state. The reduced density operator in $H_S$ is $\hat{\sigma}^S$ given by

$$
\hat{\sigma}^S = \text{Tr}_R(|\Xi_n\rangle_{RS}\langle\Xi_n|_{RS})
$$

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

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

**K.8 Irreducible Matrix Representations and Super-selection Rules**

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

$$
\hat{T}(g) |i\rangle = \sum_j D_{ji}(g) |j\rangle
$$

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

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

(239)

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

The irreducible matrices satisfy the so-called great orthogonality theorem [112]

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

(240)

The proof of this result is based on Schur’s lemma.

The importance of the irreducible representations and the consequent orthogonality theorem lies in its application to Situation B cases, where we have seen that Charlie’s density operator \( \hat{\rho} \) is invariant under any of the transformations \( \hat{T}(h) \hat{\rho} \hat{T}(h)^{-1} = \hat{\rho} \). Suppose we represent \( \hat{\rho} \) in terms of the basis vectors \( |\Gamma_\alpha \lambda \rangle \) associated with the irreducible representations

\[
\hat{\rho} = \sum_{\alpha} \sum_{\beta} R^{\alpha\beta}_{\alpha\tau} |\Gamma_\alpha \lambda \rangle \langle \Gamma_\beta \tau |
\]

(241)

where \( R \) will be a Hermitian, positive definite matrix with unit trace since it represents a density operator. Applying the transformation gives

\[
\hat{T}(h) \hat{\rho} \hat{T}(h)^{-1} = \sum_{\alpha\lambda\mu} \sum_{\beta\tau\xi} R^{\alpha\beta}_{\lambda\mu} D^\alpha_{\mu\lambda}(h) |\Gamma_\alpha \mu \rangle \langle \Gamma_\beta \xi | D^\beta_\tau(h)^* = \hat{\rho}
\]

(242)

Averaging over \( h \) and using the great orthogonality theorem gives

\[
\hat{\rho} = \sum_{\alpha} \sum_{\mu} \left( \sum_{\lambda} \frac{1}{d_\alpha} R^{\alpha\beta}_{\lambda\lambda} \right) |\Gamma_\alpha \mu \rangle \langle \Gamma_\alpha \mu |
\]

(243)

This is in the form of a mixed state involving irreducible state vectors \( |\Gamma_\alpha \mu \rangle \) each occurring with a probability \( P^\alpha_\mu \) given by

\[
P^\alpha_\mu = \sum_{\lambda} \frac{1}{d_\alpha} R^{\alpha\beta}_{\lambda\lambda} = P^\alpha
\]

(244)
which is the same for all \( \mu \) associated with a given irreducible representation \( \Gamma_\alpha \). This is clearly a positive real quantity and since

\[
\sum_\alpha \sum_\mu P_{\mu}^\alpha = \sum_\alpha \sum_\mu \sum_\lambda \frac{1}{d_\alpha} R_{\alpha \alpha}^{\alpha \lambda} = \sum_\alpha \sum_\lambda R_{\alpha \alpha}^{\alpha \lambda} = \text{Tr} \hat{\rho} = 1 \quad (245)
\]

the probabilities sum to unity as required.

The final result for Charlie’s density operator

\[
\hat{\rho} = \sum_\alpha \sum_\mu P_{\mu}^\alpha |\Gamma_\alpha \mu\rangle \langle \Gamma_\alpha \mu| \quad (246)
\]
demonstrates the presence of a super-selection rule. In Charlie’s description of the quantum state there are no coherences between states |\( \Gamma_\alpha \mu \rangle \) associated with differing irreducible representations of the transformation group. This represents the general form of the SSR for all transformation groups in Situation B cases.

As an example, consider the \( U(1) \) group and the single mode bosonic system. Since the Fock states satisfy \( \hat{T}(\theta_a) |n_a\rangle = \exp(i n_a \theta_a) |n_a\rangle \) they form the basis for the irreducible representations of the \( U(1) \) group, the occupation number \( n_a \) specifying the irreducible representation and the \( 1 \times 1 \) matrices \( \exp(i n_a \theta_a) \) being the unitary matrices. Hence Charlie will describe the quantum state as

\[
\hat{\rho} = \sum_{n_a} P(n_a) |n_a\rangle \langle n_a| \quad (247)
\]

which is a statistical mixture of Fock states with no coherences between different Fock states. This result is of the same form as in Eq. (89) and is in accord with the SSR on boson number.

As another example, consider the \( U(1) \) group and the multi-mode bosonic system. Here sums of products of Fock states

\[
|n_1 n_2 \ldots n_a \ldots; N\rangle = \prod_a |n_1\rangle |n_2\rangle \ldots |n_a\rangle \ldots \quad N = \sum_a n_a \quad (248)
\]
such that the total occupancy is \( N = \sum_a n_a \) can be used to form irreducible representations for the transformation group in terms of linear combinations of the products with the same \( N \). Writing these linear combinations as

\[
|\Psi_N^\mu\rangle = \sum_{\{n_1 n_2 \ldots n_a \ldots\}} C_{\{n_1 n_2 \ldots n_a \ldots\}}^N |n_1 n_2 \ldots n_a \ldots; N\rangle \quad (249)
\]

we have since \( \hat{T}(\theta) |n_1 n_2 \ldots n_a \ldots; N\rangle = \exp(i N \theta) |n_1 n_2 \ldots n_a \ldots; N\rangle \) we see that \( \hat{T}(\theta) |\Psi_N^\mu\rangle = \exp(i N \theta) |\Psi_N^\mu\rangle \) also, so the \( |\Psi_N^\mu\rangle \) define the irreducible basis states. The total occupancy \( N \) specifies the irreducible representation, but here there
are many irreducible representations with the same \( N \) depending on the various \( \mu \). In this case Charlie will describe the state as

\[
\hat{\rho} = \sum_{N} \sum_{\mu} P_{\mu}^{N} |\Psi_{\mu}^{N}\rangle \langle \Psi_{\mu}^{N}| \tag{250}
\]

which is a statistical mixture of multi-mode states \( |\Psi_{\mu}^{N}\rangle \) all with the same total occupancy \( N \). Although there are coherence terms between individual modal Fock states, there are no coherences between states with different total occupancy. This result is of the same form as in Eq.(62) and again is an example of a super-selection rule operating in terms of Charlie's description of the quantum state.

Finally, we note that in situation A where the relationship between the frames is known and there is no invariance for Charlie's density operator, we do not have SSR applying. For the single particle case and the translation group the momentum states \( |p\rangle \) define the irreducible representations, each specified by \( p \), and as we saw Charlie's description of the quantum state involved linear combinations of these irreducible basis vectors, in contradiction to the SSR.

### K.9 Non-Entangled States

The essential feature of an non-entangled or separable state is that the sub-systems are considered to be unrelated to each other. Hence, both for Alice and Charlie there will be separate reference frames for each sub-system, with transformation groups - \( \hat{T}_A(g_a) \) for sub-system A, \( \hat{T}_B(g_b) \) for sub-system B, etc which relate the reference systems of Alice to those of Charlie. The transformations \( g_a, g_b, \ldots \) are different. The overall transformation operator would be of the form \( \hat{T}(g_a, g_b, \ldots) = \hat{T}_A(g_a) \otimes \hat{T}_B(g_b) \otimes \ldots \). Alice would describe a general non-entangled state as having a density operator

\[
\hat{\sigma} = \sum_{R} P_{R} \hat{\sigma}_R^A \otimes \hat{\sigma}_R^B \otimes \hat{\sigma}_R^C \otimes \ldots \tag{251}
\]

It then follows for Situation B where the reference frames for Alice and Charlie are unrelated, that Charlie would describe the same state via the density operator

\[
\hat{\rho} = \sum_{R} P_{R} \hat{\rho}_R^A \otimes \hat{\rho}_R^B \otimes \hat{\rho}_R^C \otimes \ldots \tag{252}
\]

where

\[
\hat{\rho}_R^C = \int w(g_c) dg_c \hat{T}_C(g_c) \hat{\sigma}_R^C \hat{T}_C(g_c)^{-1} \quad C = A, B, \ldots \tag{253}
\]

Note that separate twirl operations are applied to the different sub-systems, as explicitly shown in the papers by Vaccaro et al [63] (see Section IIIA, Eqn. 3.3 therein) and Paterek et al [65] (see Section 6). This leads for general transformation groups to the local group super-selection rule, where the \( \hat{\rho}_R^C \) involve
no coherences between states associated with differing irreducible representations of the transformation group. We see that Charlie also describes a non-entangled state and with the same mixture probability $P_R$ as for Alice. Thus non-entanglement or separability is a feature that is the same for both Alice and Charlie, as ought to be the case.

In the context of sub-systems consisting of modes (or sets of modes) occupied by identical bosons, the case of interest is Situation B, with each transformation group being U(1). Here the relationship between Charlie’s and Alice’s phase reference frames are unknown. Hence irrespective of Alice’s description of the sub-system states $\hat{\sigma}^A_R, \hat{\sigma}^B_R, \ldots$ we see from the previous section that Charlie will describe the separate sub-system states $\hat{\rho}^A_R, \hat{\rho}^B_R$, as statistical mixtures of number states for the separate modes (or total number states for the sets of modes in each sub-system). Thus from Charlie’s point of view the separate mode density operators will satisfy the SSR. Thus we see that the introduction of reference frames and two observers - Charlie being the external one whose description of the quantum states is of primary interest - leads to the same SSR outcome as the simpler considerations set out in SubSections 3.2 and 3.4. Essentially the same considerations have been used in [54], [63] and the other papers to justify the local photon number superselection rule.

K.10 SSR Justification and Galilean Frames ?

Finally, in addition to the previous reasons there is an argument that has been proposed based on the requirement that the dynamical equations for such non-relativistic quantum systems should be invariant under a Galilean transformation which has been proposed [103] as a proof of the super-selection rule for atom number. This approach is linked to the reference frame based justification of SSR described in this Appendix. However, whilst the paper shows that under a Galilean transformation - corresponding to describing the system from the point of view of an observer moving with a constant velocity $v$ with respect to the original observer, and where the two observers have identical clocks - the terms in a superposition state with different numbers $N$ of massive bosons would oscillate like $\exp i \left( \frac{1}{2} Nmv^2 t / \hbar \right)$, and may be expected if the same quantum state is described by a moving observer. This feature alone does not seem to require the super-selection rule, since here the moving observer’s reference frame has a well-defined velocity with respect to that attached to the system. However, the moving observer’s reference frame may actually have an unknown relative velocity, in which case a twirling operation resulting in the elimination of number state coherences could be involved (see Appendix K). This will be not be considered further at this stage.

On the other hand, an approach of this kind involving rotation symmetry would seem to rule out such states as quantum superpositions of a boson (spin 0) and a fermion (spin 1/2). Let such a state be prepared in the form $\left( |F\rangle + |B\rangle \right) / \sqrt{2}$. Consider an observer whose Cartesian reference frame is $X, Y, Z$. This is a classical system that can be rotated in space. If the observer rotates with his frame through $2\pi$ about any axis they are then back in the same position,
but the observer now sees the state as \((-|F\rangle + |B\rangle)/\sqrt{2}\). This state is apparently orthogonal to the one observed before the rotation, and this is paradoxical since the observer would be in the same position. Thus there is a super-selection rule excluding states such as \((|F\rangle + |B\rangle)/\sqrt{2}\). A similar argument based on the time reversal anti-unitary operator was given by Wick et al [59].
Appendix L  SSR and Photons

Though this paper is focused on massive bosonic atoms the question is whether similar SSR also apply to the optical quantum EM field, which involve massless bosons - photons. Here the situation is not so clear and we therefore merely present the differing viewpoints in the current literature. Some of the same general reasons for applying the super-selection rule to systems of identical massive bosons also apply here, though the details differ, but others do not. The situation depends also on whether optical or microwave photons are involved. The issue is whether for individual photon modes, states can be prepared that are not local particle number SSR compliant, and if so can the effects of the non-SSR compliant terms be observed and furthermore do we need to invoke the existence of non SSR compliant states to understand interference and coherence effects. As we will see, some SSR non compliant feature needs to be present in order to prepared allegedly non SSR compliant states. Another way of looking at the issue is to ask whether phase reference systems exist for photon modes. In addition, there is the issue for multi-mode situations whether states can be prepared, observed or are needed that are not global particle number SSR compliant. As we will see, SSR may now involve a modified total particle number involving combinations of the mode numbers different to the total particle number - because it is these combinations that are conserved in mode interaction processes. In the approach adopted in this paper, the states in question are those described by so-called external observers - not hypothetical observers that are somehow attached to phase reference systems internal to the experiment (see below, Section 3.3). The SSR issue for systems involving massless photons is particularly important in regard to describing entanglement. As explained below in Section 3.4, if separate sub-system states in photonic systems can be prepared with density operators that violate the local particle number SSR, then these so-called “separable but non-local” states [56] would be classified as separable rather than as entangled states. Some of the tests for entanglement described in Paper II for systems of massive boson (such as spin squeezing in any spin component) would then no longer apply for photonic systems, though others (such as the Hillery spin variance test) which do not depend on SSR would still apply.

We first consider the requirement of showing how a non SSR compliant states can be prepared for single modes. In the case of photons, Mølmer [113] has argued that the quantum state for a single mode optical laser field operating well above threshold is not a Glauber coherent state, and the density operator would be a statistical mixture of the form (62), with $|\Phi_N\rangle = |N\rangle$ and $P_{\Phi_N} = \exp(-N) / N!$. Here the density operator is a statistical mixture of photon number states with a Poisson distribution, or equivalently a statistical mixture of equal amplitude coherent states $|\alpha\rangle$ with $\alpha = \sqrt{N} \exp(i\phi)$ and all phases $\phi$ having equal probability. In either form, the quantum state is SSR compliant. In terms of possible processes for preparing states for single mode optical laser fields, this feature is confirmed in theories for single mode
lasers involving atomic gain media energized via incoherent pumping processes - there is no well defined optical phase that is imposed on the process. The Scully-Lamb theory (see Mandel and Wolf [114], p935) gives the above threshold steady state density operator for the laser mode can be written in the form of a statistical mixture of number states (somewhat broader than for a Poisson distribution), which again is an SSR compliant state with no well-defined optical phase. Further detailed discussion of laser light generation processes by Pegg and Jeffers [82] confirms this. An alternative approach is presented by Wiseman et al [115], [116], in which the optical laser is treated via a master equation, but where monitoring of the laser environment (difficult!) is required to determine whether certain pure state ensembles - such as those involving coherent states - are physically realizable. The assumed monitoring assumes the presence of another phase reference. The conclusion reached is that for finite self energy the coherent state ensemble is not physically realizable, the closest ensemble being that involving squeezed states, though for zero self energy coherent state ensembles are obtained. On the other hand, microwave photons in single mode high Q cavities can be generated by oscillating electric currents having a well-defined phase. In this case, as shown in experiments on the Jaynes-Cummings model by Rempe et al [117] and Brune et al [118] demonstrating collapses and revivals of Rydberg atom population differences, it is possible to create Glauber coherent states in microwave cavity modes, and the presence of these states are necessary to explain the collapse and revival effects.

We next consider cases where interacting photon modes are involved. The two mode squeezed states generated for example in a non-degenerate parametric amplifier are often written in the form $\sum_n C_n |n\rangle_A |n\rangle_B$, corresponding to the basic generation process in which a pump photon of frequency $\omega_C = \omega_A + \omega_B$ is destroyed and one photon is created in each of modes $A$ and $B$. Such a state is not even global SSR compliant, but is used in describing various quantum information processes as well as describing two mode squeezing. However, whilst mathematically convenient for treating such applications this do not demonstrate that this two mode pure state has actually been created. This state vector is in fact based on a very simplified version of the process, in which the pump mode is treated classically. If it is treated quantum mechanically and there were $N$ photons initially in mode $C$, the interaction term $\hat{V} = \lambda \hat{a}^\dagger \hat{b}^\dagger + HC$ would result in a global SSR compliant state vector like $\sum_n C_n |N-n\rangle_C |n\rangle_A |n\rangle_B$, but now involving a total quanta number $\hat{N}_{tot} = \hat{N}_A + \hat{N}_B + 2\hat{N}_C$ (see Section 3.2.3 for details). The state describing modes $A$ and $B$ alone would be $\hat{\rho}_{AB} = \sum_n |C_n|^2 |n\rangle_A \langle n| \otimes |n\rangle_B \langle n|_B$. This state is global SSR compliant in terms of $\hat{N}_{A,B} = \hat{N}_A + \hat{N}_B$ but is not the same as the pure state $\sum_n C_n |n\rangle_A |n\rangle_B$ - which is not SSR compliant. Even more elaborate quantum treatments allowing for irreversible damping processes for all three modes (see for example McNeil et al [119]) that result in non SSR compliant steady state solutions, include assumptions such as the pump mode being coupled to a laser mode.
that is treated classically - and thus begging the question of whether non SSR compliant states were prepared, since the classical treatment of the laser mode is itself SSR non compliant. We are unaware of any situation where non SSR compliant states are claimed to have been created for optical photons, where the theoretical treatment of the preparation process has not assumed the presence of non SSR compliant states for some key sub-system involved - usually in an input pump mode. In Section 3.2.3 we considered a preparation process for the non-degenerate parametric amplifier involving conservation of $\hat{N}_{\text{tot}}$ starting from an initial separable state in which all the sub-system density operators are local particle number SSR compliant and show that this results in a quantum state that is global SSR compliant in terms of total quanta number $\hat{N}_{\text{tot}}$. There must therefore be some non SSR compliant feature in the initial state (which could include pump modes) to produce global non SSR compliant states, so then the issue shifts back to how these non SSR compliant states are prepared in the first place.

Second, there is the requirement of being able to measure the non SSR compliant terms. For the free quantum EM field there is a conservation law for the photon number in each mode, so in a pure state such as in Eq. (61) the $|C_N|^2$ would be time independent. However, for photons the $C_N$ would oscillate with frequencies that only differ by non-relativistic photon frequencies rather than the Compton frequency that applies for massive bosons, so the argument against being able to detect coherent states based on this frequency being so large that the oscillations cannot be followed do not necessarily apply. Clocks that enable oscillations in microwave fields to be followed are common-place, and the recent development of clocks with shorter time scales may enable oscillations of optical fields to be observed. So this consideration does not rule out non SSR compliant states, even for optical photons.

Finally, we consider the requirement of non SSR compliant states being needed to explain interference, coherence effects etc. We need to distinguish the situation where it is mathematically convenient to invoke SSR non compliant states to explain these effects from the situation where it is essential to do so. Thus it may be convenient to explain the presence of interference patterns in position measurements for bosons from two independent BECs by choosing Glauber coherent states to represent their states, but as pointed out in Section 3.2.5 such interference patterns are accounted in terms of Fock states, together with quantum interference of probability amplitudes associated with bosons being taken from the two different sources (see Refs. [105], [68], [102]). In fact, the more detailed feature that although the separation of the peaks is well defined the actual position of the peaks are random, is inconsistent with the Glauber coherent state description. We also point out below (see Section 3.3.2 and Appendix M) that the interpretation of Ramsey fringes in a proposed experiment to detect a coherent superposition of an atom and a molecule does not show that such a state was created or that the BEC involved had to be described by a Glauber coherent state. Many experiments in which coherence, interference effects are observed do not depend on SSR non compliant states being created. Optical interference and coherence effects can also be explained
without invoking Glauber coherent states, as shown by Mølmer [113] and in other papers such as [68]. In regard to two mode squeezing in the non-degenerate parametric amplifier described above, the observation of squeezing effects is often discussed in terms of SSR non-compliant states of the form \( \sum_n C_n |n\rangle_A |n\rangle_B \) (see Ref. [19] for example). However, as may be seen from the experimental paper of Ou et al [120], the way in which two mode squeezing is observed in the non-degenerate parametric amplifier involves generating the pump field by frequency doubling from a lower frequency laser. That lower frequency laser is also used to provide the local oscillator fields for the homodyne measurements on modes \( A \) and \( B \) used to detect squeezing - these modes are coupled to the local oscillator fields using beam splitters. The original lower frequency laser acts as an internal phase reference for the overall experiment, as may be seen in Fig 2 of Ref [120] which involves the relative phase between the local oscillator and the squeezed input field. But as there is no external phase reference system involved, only the relative phases of the \( A \) and \( B \) modes are well defined, and not the overall phase as would be required for preparing non SSR compliant states. Again the convenient use of SSR non-compliant states to understand experiments in which only internal phase references are involved does not show that SSR non-compliant states are necessary to interpret the experiments. A similar arrangement occurs for the degenerate parametric amplifier experiment of Wu et al [121], where Fig 2 clearly shows how the local oscillator field derives from the original Nd-YAG laser. The role that a laser may play as a clock and in establishing an internal phase reference in such experiments is carefully discussed by Wiseman [122].

Perhaps the best way to approach the question of whether SSR compliance is required for optical photons for example (see SubSection 3.3 and SubSection K.4 in Appendix K) involves the consideration of phase reference frames. The quantum state of a single mode laser may be described as a Glauber coherent state by an observer (Alice) with one reference frame, but would be described as a statistical mixture of photon number states by another observer (Charlie) with a different reference frame whose phase reference is completely unrelated to the previous one. This argument against the presence of coherent state in Charlie’s viewpoint is only overcome if inter-related phase reference frames at the relevant photon frequencies actually exist.
Appendix M  Super-Selection Rule Violations

M.1  Preparation of Coherent Superposition of an Atom and a Molecule

A key paper dealing with the coherent superposition of an atom and a molecule is that by Dowling et al [106], entitled “Observing a coherent superposition of an atom and a molecule”. Essentially the process involves one atom A interacting with a BEC of different atoms B leading to the creation of one molecule AB, with the BEC being depleted by one B atom.

M.1.1  Hamiltonian

The Hamiltonian is given by

\[ \hat{H} = \hbar \omega_A \hat{b}_A^\dagger \hat{b}_A + \hbar \omega_M \hat{b}_M^\dagger \hat{b}_M + \hbar \omega_2 \hat{b}_2^\dagger \hat{b}_2 + \frac{\hbar \kappa}{2} (\hat{b}_M^\dagger \hat{b}_A \hat{b}_2 + \hat{b}_M \hat{b}_A^\dagger \hat{b}_2^\dagger) \]  

(254)

where \( \hat{b}_A, \hat{b}_M \) and \( \hat{b}_2 \) are standard bosonic annihilation operators for the atom, molecule and BEC modes respectively, \( \omega_A, \omega_M \) and \( \omega_2 \) are the corresponding mode frequencies and \( \kappa \) defines the interaction strength for the process where a molecule is created or destroyed from/to an atom A and a BEC atom B. \( \Delta \) is the frequency difference between the molecular state AB and the two separate states for atoms A and B – this is zero on Feshbach resonance - and is given by

\[ \Delta = \omega_M - \omega_A - \omega_2 \]  

(255)

The Hamiltonian commutes with the total number operator \( \hat{N}_{tot} \), where

\[ \hat{N}_{tot} = 2 \hat{b}_M^\dagger \hat{b}_M + \hat{b}_A^\dagger \hat{b}_A + \hat{b}_2^\dagger \hat{b}_2 \]  

(256)

where the molecule number operator is multiplied by two.

M.1.2  Initial State

Initially the state of the system is given by the density operator Eqs (10) and (11) in the paper

\[ \hat{W}_{0L} = \int \frac{d\theta}{2\pi} \exp(-i\hat{N}_{tot}\theta) |\Psi\rangle_{0L} \langle \Psi|_{0L} \exp(+i\hat{N}_{tot}\theta) \]  

(257)

\[ |\Psi\rangle_{0L} = |A\rangle |\beta\rangle \]  

(258)

where \( |A\rangle \) is a state with one atom A and \( |\beta\rangle \) is a Glauber coherent state for the BEC of atoms B. The super-operator acting on the pure state \( |\Psi\rangle_{0L} \langle \Psi|_{0L} \) is called the twirling operator, the group of unitary operators \( \exp(-i\hat{N}_{tot}\theta) \) depend on a phase variable \( \theta \) and are a unitary representation of \( U(1) \), the generator
being $\hat{N}_\text{tot}$. These operators act as a symmetry group for the system and leave the Hamiltonian invariant. The initial state is also given by

$$\hat{W}_L(0) = \hat{\rho}_{A-M}(0) \otimes \hat{\rho}_2(0)$$  \hspace{1cm} (259)

$$\hat{\rho}_{A-M}(0) = |A\rangle \langle A|$$  \hspace{1cm} (260)

$$\hat{\rho}_2(0) = \int \frac{d\theta}{2\pi} \exp(-i\hat{n}_2\theta) |\beta\rangle \langle \beta| \exp(+i\hat{n}_2\theta)$$  \hspace{1cm} (261)

$$= \sum_n p_n(< n > |n\rangle \langle n|$$  \hspace{1cm} (262)

$$= \int \frac{d\theta}{2\pi} |\beta\rangle \langle \beta| \exp(-i\theta) \langle \beta| \exp(-i\theta)|$$  \hspace{1cm} (263)

where $\hat{n}_2 = \hat{b}_2\hat{b}_2$ is the number operator for the BEC mode and $p_n(< n >) = \{\exp(-< n > < n >^n / n!\}$ is a Poisson distribution, whose mean is $< n > = |\beta|^2$. Initially then there is one atom A and the BEC is in a statistical mixture of number states with a Poisson distribution, which is mathematically equivalent to a statistical mixture of Glauber coherent states $|\beta\rangle \exp(-i\theta)$ with the same amplitude $\sqrt{< n >}$ but with all phases (arg $\beta + \theta$) being equally weighted.

**M.1.3 Implicated Reference Frame**

In the paper by Dowling et al [106] the BEC is acting as an implicated phase reference frame (see [71], [60]). The state of the reference frame as described by Charlie is given by

$$\hat{\rho}_{\text{REF}} = \hat{\rho}_2(0) = \int \frac{d\theta}{2\pi} \exp(-i\hat{n}_2\theta) |\beta\rangle \langle \beta| \exp(+i\hat{n}_2\theta)$$  \hspace{1cm} (264)

and from Eq. (254), there is an interaction between the reference BEC and the separate atom A and molecule M systems. However, because $< n > = |\beta|^2$ is very large, the BEC is essentially unchanged during the process, as reflected in the use of approximations in Eqs (27), (28) of the paper. Another implicated phase reference frame situation, but involving a two mode reference frame is discussed in the paper by Paterek et al [65]

Overall, in terms of the discussion in Appendix K $\hat{W}_L$ would be Charlie’s description of the initial state, whereas Alice would describe it as $|\Psi\rangle_{0L} \langle \Psi|_{0L}$. Presumably in the paper by Dowling et al [106] what is referred to as the “state of the laboratory” be Charlie’s reference frame, and what they refer to as the “internal reference frame” would refer to that of Alice. However, whether Alice could actually prepare such a state as $|\Psi\rangle_{0L} \langle \Psi|_{0L}$ is controversial - see SubSections 3.2 and 3.4, though here this is assumed to be possible.

**M.1.4 Process - Alice and Charlie Descriptions**

There are three stages in the process, the first being with the interaction that turns separate atoms A and B into the molecule AB turned on at Feshbach
resonance for a time \( t = \pi/(2\kappa < n >) \), the second being free evolution at large Feshbach detuning \( \Delta \) for a time \( \tau \) leading to a phase factor \( \phi = \Delta \tau \), the third being again with the interaction turned on at Feshbach resonance for a further time \( t = \pi/(2\kappa < n >) \). The typical initial state \( |\Psi_{0L}\rangle \) given by \( |A\rangle |\beta\rangle \) (Eq (11)) evolves into \( |\Psi_{3L}\rangle \) given by (see Eq. (32) of paper)

\[
|\Psi_{3L}\rangle = \left( \sin\left(\frac{\phi}{2}\right) |A\rangle - \exp(i \arg \beta) \cos\left(\frac{\phi}{2}\right) |M\rangle \right) |\beta\rangle
\]

using approximations set out in Eqs (27), (28) of the paper that depend on \( < n > \) being large. Here \( |M\rangle \) is a state with one molecule AB. Thus it looks like a coherent superposition of an atom state \( |A\rangle \) and a molecule state \( |M\rangle \) has been prepared, the atom plus molecule system being disentangled from the BEC. Alice would describe the final state of the system as \( |\Psi_{3L}\rangle \langle \Psi_{3L}| \), so from her point of view a coherent superposition of an atom and a molecule has been prepared.

However, for Charlie the final state of the system is described by a density operator \( \hat{W}_{3L} \) which is reconstructed by applying the twirling operator to \( |\Psi_{3L}\rangle \langle \Psi_{3L}| \). Noting that

\[
\exp(-i \hat{N}_{\text{tot}} \theta) |\Psi_{3L}\rangle = \left( \exp(-i \theta) \sin\left(\frac{\phi}{2}\right) |A\rangle - \exp(-2i \theta) \exp(i \arg \beta) \cos\left(\frac{\phi}{2}\right) |M\rangle \right) |\beta\rangle
\]

we see that Charlie’s final reduced density operator for the atom-molecule system is

\[
\hat{\rho}_{A-M}(3) = Tr_2 \hat{W}_{3L} = Tr_2 \int \frac{d\theta}{2\pi} \exp(-i \hat{N}_{\text{tot}} \theta) |\Psi_{3L}\rangle \langle \Psi_{3L}| \exp(+i \hat{N}_{\text{tot}} \theta)
\]

\[
= \int \frac{d\theta}{2\pi} \left( \exp(-i \theta) \sin\left(\frac{\phi}{2}\right) |A\rangle - \exp(-2i \theta) \exp(i \arg \beta) \cos\left(\frac{\phi}{2}\right) |M\rangle \right) \times \left( \exp(+i \theta) \sin\left(\frac{\phi}{2}\right) \langle A| - \exp(+2i \theta) \exp(-i \arg \beta) \cos\left(\frac{\phi}{2}\right) \langle M| \right)
\]

\[
= \sin^2\left(\frac{\phi}{2}\right) |A\rangle \langle A| + \cos^2\left(\frac{\phi}{2}\right) |M\rangle \langle M|
\]

Thus the coherence terms like \(|A\rangle \langle M|\) and \(|M\rangle \langle A|\) do not appear in the final density operator when the average over \( \theta \) (not \( \beta \)) is carried out.

For Charlie the density operator for the atom and molecule is of course a statistical mixture of a state with one atom and no molecule and a state with no atom and one molecule. The authors of [106] actually point this out in the paragraph after Eq (35) where (presumably for the case \( \phi = \pi/4 \)) it is
stated “the state is found to be ... an incoherent mixture of an atom and a molecule.”. The probabilities for detecting an atom A or a molecule AB are as in Eq (33) of the paper. In terms of Charlie’s description, the density operator at the end of the preparation process does not signify the existence of a coherent superposition of an atom and a molecule, as the title to the paper might be taken to imply. The existence of such a coherent superposition would of course be present in Alice’s description, but it is Charlie’s (laboratory) description that is more relevant.

M.1.5 Interference Effects Without SSR Violation

Note that interference effects are still present since the atom or molecule detection probabilities depend on the phase $\phi$ associated with the free evolution stage of the process. However, as in many other instances, the presence of coherence effects does not require the existence of coherent superposition states that violate the super-selection rule. The authors actually point this out in the paragraph after Eq (35), where it is stated “we have clearly predicted the standard operational signature of coherence, namely Ramsey type fringes, but the coherence is not present in our mathematical description of the system.” What they are referring to is Charlie’s description of the final state - which indeed shows no such coherence, but the belief that coherent superposition states are needed to predict coherence effects is mistaken.

To drive this point home, the process can be treated with the initial state for the BEC being given as a Fock state $|N\rangle$. With the interaction being given as in Eq.(254) (Eq (14) in the paper) the state vector is a simple linear combination of two terms

$$|\Psi(t)\rangle = A(t) |A\rangle |N\rangle + B(t) |M\rangle |N-1\rangle$$

(269)

This is of course an entangled state. Coupled equations for the two amplitudes $A(t)$ and $B(t)$ can easily be obtained and simple solutions obtained for stages where the Feshbach detuning is either zero or large. The state vector is continuous from one stage to the next, and the reduced density operator at the end of the three stage process for the atom plus molecule sub-system can be obtained. It is of the form

$$\hat{\rho}_{A-M}(3) = Tr_2(|\Psi(3)\rangle \langle \Psi(3)|)$$

$$= \sin^2(\frac{\phi}{2}) |A\rangle \langle A| + \cos^2(\frac{\phi}{2}) |M\rangle \langle M|$$

(270)

which is of course a statistical mixture of a state with one atom and no molecule and a state with no atom and one molecule - and is exactly the same result as obtained in the paper by Dowling et al.[106]. Note that coherence effects in regard to the interferometric dependence on $\phi$ for measurements on the final state has been found without invoking either the description of the BEC via Glauber coherent states or the presence of a coherent superposition of an atomic and a molecular state. The result can easily be extended for the case where the BEC is initially in a statistical mixture of Fock states with differing $N$ occurring.
with a probability \( P_N \). Each initial state \( |A⟩|N⟩ \) evolves as in Eq. (269). We then would have
\[
\hat{\rho}_{A-M}(3) = Tr_2 \left( \sum_N P_N |\Psi_N(3)⟩⟨\Psi_N(3)| \right)
\]
\[
= \sum_N P_N \left( \sin^2 \left( \frac{\phi}{2} \right) |A⟩⟨A| + \cos^2 \left( \frac{\phi}{2} \right) |M⟩⟨M| \right)
\]
\[
= \sin^2 \left( \frac{\phi}{2} \right) |A⟩⟨A| + \cos^2 \left( \frac{\phi}{2} \right) |M⟩⟨M| \quad (271)
\]
which is the same as before. Allowing for a statistical mixture of Fock states makes no difference to the interferometric result.

M.1.6 Conclusion

Dowling et al [106] state in their abstract that “we demonstrate that it is possible to perform a Ramsey-type interference experiment to exhibit a coherent superposition of a single atom and a diatomic molecule”. However the interferometric effects (involving the dependence on \( \phi \)) cannot be said to exhibit the existence of such a coherent superposition, since the same interferometric results can be obtained without ever introducing such a quantum state. There is not a convincing case that quantum states that violate the super-selection rule forbidding the creation of coherent superpositions of Fock states with differing particle numbers can be created, even in Alice’s reference system. The fact that an SSR violating state \( |Ψ⟩_3L \langle Ψ|_3L \) is created in Alice’s reference system is not surprising, because in the process considered the initial state \( |β⟩ \) for the BEC was assumed as a factor in Alice’s initial state, and this was itself inconsistent with the SSR. Furthermore, such SSR violating states are not needed to describe coherence and interference effects, so that justification for their physical existence also fails.

M.2 Detection of Coherent Superposition of a Vacuum and a One-Boson State?

Whether such super-selection rule violating states can be detected has also not been justified. For example, consider the state given by a superposition of a one boson state and the vacuum state (as discussed in [107]). Consider an interferometric process in which one mode \( A \) for a two mode BEC interferometer is initially in the state \( |0⟩ + |1⟩ \), and the other mode \( B \) is initially in the state \( |0⟩ \) - thus \( |Ψ(i)⟩ = (α |0⟩ + β |1⟩)_A ⊗ |0⟩_B \) in the usual occupancy number notation, where \( |α|^2 + |β|^2 = 1 \). Modes \( A, B \) could refer to two different hyperfine states of a bosonic atom with non-relativistic energies \( \hbar ω_A \) and \( \hbar ω_B \), mode annihilation operators \( \hat{a}, \hat{b} \). The modes are first coupled by a beam splitter, which could be a resonant microwave pulse that causes transitions between the two hyperfine
states and which can be described via a unitary operator $\hat{U}_{BS}$ such that

$$\hat{U}_{BS}(|1\rangle_A \otimes |0\rangle_B) = (|1\rangle_A \otimes |0\rangle_B - i |0\rangle_A \otimes |1\rangle_B)/\sqrt{2}$$

$$\hat{U}_{BS}(|0\rangle_A \otimes |1\rangle_B) = (-i |1\rangle_A \otimes |0\rangle_B + |0\rangle_A \otimes |1\rangle_B)/\sqrt{2}$$

$$\hat{U}_{BS}(|0\rangle_A \otimes |0\rangle_B) = (|0\rangle_A \otimes |0\rangle_B).$$  \hspace{1cm} (272)

After passing through the beam splitter the system is allowed to evolve freely for a time $\tau$, the Hamiltonian being

$$\hat{H}_{\text{free}} = (mc^2 + \hbar \omega_A)\hat{a}^{\dagger}\hat{a} + (mc^2 + \hbar \omega_B)\hat{b}^{\dagger}\hat{b}$$

where collisional effects have been ignored and the rest mass energy included for completeness. Following the free evolution stage, the modes are then coupled again via a beam splitter, and the probability of an atom being found in modes $A, B$ then being measured. A straightforward treatment of the evolution shows that the final state is given by

$$|\Psi(f)\rangle = \alpha(|0\rangle_A \otimes |0\rangle_B) + \beta \exp(-i\{mc^2/\hbar + \omega_A\} \tau) \times \left( \frac{1 - \exp(-i\Delta\tau)}{2} (|1\rangle_A \otimes |0\rangle_B) - i \frac{1 + \exp(-i\Delta\tau)}{2} (|0\rangle_A \otimes |1\rangle_B) \right)$$

\hspace{1cm} (273)

where $\Delta = \omega_B - \omega_A$ is the detuning. The probabilities of finding one atom in modes $A, B$ respectively are

$$P_{10} = |\beta|^2 \sin^2(\Delta\tau/2) \quad P_{01} = |\beta|^2 \cos^2(\Delta\tau/2)$$  \hspace{1cm} (274)

Thus whilst coherence effects occur depending on the phase difference $\phi = \Delta\tau$ associated with the interferometric process, the overall detection probabilities only depend on the initial state via $|\beta|^2$. There is no dependence on the relative phase between $\alpha$ and $\beta$, as would be required if the superposition state $\alpha |0\rangle + \beta |1\rangle$ is to be specified from the measurement results. Exactly the same detection probabilities are obtained if the initial state is the mixed state $\hat{\rho}(i) = |\alpha|^2(|0\rangle_A \langle 0|_A \otimes |0\rangle_B \langle 0|_B) + |\beta|^2(|1\rangle_A \langle 1|_A \otimes |0\rangle_B \langle 0|_B)$, 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 coherent superposition associated with the super-selection rule violating state would not be detected in the interferometric process. The paper by Dunningham et al \cite{107} considers first a detection process that involves using a Glauber coherent state as one of the input states. Similar interference effects as in Eq. (274) are obtained. A second detection process in which the single term Glauber coherent state is replaced by a statistical mixture with all phases equally weighted in considered next, leading to the same interference effects. This again confirms that it is not necessary to invoke the existence of coherent superpositions of number states in order to demonstrate interference effects.
Appendix N  Criterion for Local and Global SSR in Separable 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 $\hat{\rho}_a^R, \hat{\rho}_b^R$ to be global particle number SSR compliant is that all such sub-system states are local particle number SSR compliant.

We first note that

$$[\hat{N}, \hat{\rho}] = \sum_R P_R([\hat{n}_a, \hat{\rho}_a^R] \otimes \hat{\rho}_b^R + \hat{\rho}_a^R \otimes [\hat{n}_b, \hat{\rho}_b^R])$$  \hspace{1cm} (275)

**Necessity:** If the state $\hat{\rho}$ is globally SSR compliant then $[\hat{N}, \hat{\rho}] = 0$. Taking the trace of both sides of (275) over sub-system space $b$, using $\text{Tr}_b(\hat{\rho}_b^R) = 1$ and $\text{Tr}_b([\hat{n}_b, \hat{\rho}_b^R]) = 0$ and then repeating the process for sub-system space $a$ gives

$$0 = \sum_R P_R([\hat{n}_a, \hat{\rho}_a^R]) \hspace{1cm} 0 = \sum_R P_R([\hat{n}_b, \hat{\rho}_b^R])$$  \hspace{1cm} (276)

which are operator equation in sub-system spaces $a$ and $b$ respectively.

The $P_R$ are not independent, satisfying $\sum_R P_R = 1$. By choosing a particular $P_S$ we can write the last equation for sub-system $a$ as

$$0 = \sum_{R \neq S} P_R([\hat{n}_a, \hat{\rho}_a^R]) + (1 - \sum_{R \neq S} P_R)([\hat{n}_a, \hat{\rho}_S^a])$$  \hspace{1cm} (277)

where the remaining $P_R$ are now independent. Differentiating the last equation with respect to $P_R$ then gives

$$0 = [\hat{n}_a, \hat{\rho}_S^a] - [\hat{n}_a, \hat{\rho}_R^a]$$  \hspace{1cm} (278)

for any two different $R$ and $S$. Thus all the $[\hat{n}_a, \hat{\rho}_R^a]$ must be the same. Using $0 = \sum_R P_R([\hat{n}_a, \hat{\rho}_R^a])$ again with equal $[\hat{n}_a, \hat{\rho}_R^a]$ and $\sum_R P_R = 1$ we then see that all $[\hat{n}_a, \hat{\rho}_R^a]$ must be zero. Similar considerations show that $[\hat{n}_b, \hat{\rho}_R^b] = 0$.

As these results apply for any choice of the $P_R$ and of the $\hat{\rho}^a_R, \hat{\rho}^b_R$ we can then conclude that

$$[\hat{n}_a, \hat{\rho}_R^a] = 0 \hspace{1cm} [\hat{n}_b, \hat{\rho}_R^b]$$  \hspace{1cm} (279)

which establishes that the sub-system states are local particle number SSR compliant.

Note that the proof depended on the choice of the $P_R$ being arbitrary apart from $\sum_R P_R = 1$. If the $P_R$ are fixed then although we can show that $0 = \sum_R P_R = 1$, the conclusion remains valid.
\[ \sum_R P_R(\hat{n}_a, \hat{\rho}_R^a) = \sum_R P_R(\hat{n}_b, \hat{\rho}_R^b) \], the steps leading to \([\hat{n}_a, \hat{\rho}_R^a] = [\hat{n}_b, \hat{\rho}_R^b] = 0\) do not follow. The four sub-system states in Section 3.4.2 where all \(P_R = 1/4\) are not local particle number SSR compliant even though the overall state is global particle number SSR compliant. This would not be the case if any of the \(P_R\) differed from 1/4.

**Sufficiency**: If the sub-system states are local particle number SSR compliant then \([\hat{n}_a, \hat{\rho}_R^a] = [\hat{n}_b, \hat{\rho}_R^b] = 0\). It then follows from (275) that

\[ [\hat{N}, \hat{\rho}] = 0 \] (280)

which establishes that the separable state is global particle number SSR compliant. This conclusion applies for arbitrary \(P_R\).

**References**


