Identification of Entanglement in Ideal Quantum Systems

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A Thesis submitted to the

Department of Physics
Nuclear & Particle Physics Section

in partial fulfillment of the requirements
for the Degree of

Master of Science

in the

National & Kapodistrian University of Athens
under the supervision of

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Athens, 2013

Abstract

In this thesis, we study the notion of Quantum Entanglement mainly in the context of Quantum Information Theory, and for that purpose we have divided the content into four parts. Part I reviews all the necessary formalism of Quantum Theory, mainly regarding the density matrix formalism and generalized measurement theory, in order to prepare the reader for the next chapters. In Part II we review discrete-variable (D.V.) entanglement, namely its definition and ways to detect, quantify and concentrate it. We have included an extensive discussion on Bell's inequalities, due to their significance, and have also proposed a simple home experiment with coins to show the reader, in a more direct and comprehensible way, that a violation of these inequalities is impossible for classical objects. In Part III, we review continuous-variable (C.V.) entanglement, criteria to detect it and all the necessary formalism required to describe it. In the fourth, and last, part we use all those tools we introduced in the previous parts to study a more complicated physical system, the free non-relativistic bosonic field at finite temperature. The entanglement criteria introduced in Part III are used in order to detect spatial entanglement (i.e. non-local particle number correlations between two non-overlapping spatial regions of the field) which is of continuous variable nature. Since, in quantum information, entangled qubits (quantum two-level systems) play an indispensable role, our next goal is to extract the entanglement of the field using two qubits, using an experimentally feasible interaction Hamiltonian that was recently proposed in the literature. Indeed, we let two spatially localized, and initially independent, qubits to locally interact with the spatial degrees of freedom of the field but not with each other. The interaction lasts only for a short time, and at the end of it we quantify the entanglement of the qubits using the machinery introduced in Part II. Surprisingly, we find the two qubits to be entangled, even though they never interacted with each other and, also, even though they could be in spacelike separated regions in spacetime during the interaction. What we have accomplished, is to extract C.V. entanglement from the field and convert into D.V entanglement of the qubits. The amount of the latter is found to match exactly the amount of the violation of the C.V. separability criterion applied to the field. Finally, we found that, in the short interaction time we considered, entanglement can be extracted only if the field's temperature is lower than its critical temperature, and very close to the absolute zero. Hence, the condensation phenomenon of the field is seen to enhance the extraction of entanglement.

KEYWORDS: quantum, information, entanglement, field, extraction

Περίληψη

Σε αυτή τη διπλωματική, μελετάμε την έννοια του Κβαντικού Εναγκαλισμού κυρίως στα πλαίσια της Κβαντικής Πληροφορίας, και για το σκοπό αυτό έχουμε χωρίσει το περιεχόμενο σε τέσσερα μέρη. Στο Μέρος I γίνεται ανασκόπηση όλου του απαραίτητου φορμαλισμού της Κβαντικής Θεωρίας, κυρίως όσον αφορά το φορμαλισμό της μήτρας πυκνότητας και της θεωρίας γενικευμένης μέτρησης, με σκοπό να προετοιμάσουμε τον αναγνώστη για τα επόμενα κεφάλαια. Στο Μέρος II μελετάμε τον εναγκαλισμό σε διακριτές μεταβλητές (Δ.Μ), κυρίως τον ορισμό του και τρόπους ανίχνευσης, ποσοτικοποίησης και συγκέντρωσής του. Έχουμε συμπεριλάβει μία εκτενή συζήτηση πάνω στις ανισότητες Bell, κυρίως λόγω της σημαντικότητάς τους, κι επίσης προτείνουμε ένα απλό πείραμα 'για το σπίτι' με νομίσματα ώστε να δείξουμε στον αναγνώστη, με έναν πιο ευθύ και κατανοητό τρόπο, ότι η παραβίαση αυτών των ανισοτήτων είναι αδύνατη για κλασικά αντικείμενα. Στο Μέρος III, μελετάμε τον εναγκαλισμό σε συνεχείς μεταβλητές, κριτήρια για την ανίχνευσή του και όλο τον απαραίτητο φορμαλισμό που είναι απαραίτητος για την περιγραφή του. Τέλος, στο Μέρος I", χρησιμοποιούμε τα περισσότερα από τα εργαλεία που εισάγαμε στα προηγούμενα μέρη για να μελετήσουμε ένα πιο πολύπλοκο φυσικό σύστημα, το ελεύθερο μη-σχετικιστικό μποζονικό πεδίο σε πεπερασμένη θερμοκρασία. Τα κριτήρια εναγκαλισμού Σ.Μ. που εισάγαμε στο Μέρος III χρησιμοποιούνται για την ανίχνευση του χωρικού εναγκαλισμού (δηλ. μη-τοπικές συσχετίσεις του αριθμού σωματιδίων μεταξύ δύο μη-επικαλυπτόμενων χωρικών περιοχών του πεδίου) ο οποίος είναι τύπου συνεχών μεταβλητών. Εφόσον, στην κβαντική πληροφορία, τα εναγκαλισμένα κβαντικά bit (qubits-κβαντικά συστήματα δύο καταστάσεων) παίζουν πολύ σημαντικό ρόλο, το επόμενο μας βήμα είναι να εξάγουμε το χωρικό εναγκαλισμό του πεδίου χρησιμοποιώντας δύο qubits, μέσω μιας πειραματικά πραγματικοποιήσιμης Χαμιλτονιανής αλληλεπίδρασης που πρόσφατα προτάθηκε στη βιβλιογραφία. Έτσι, λοιπόν, αφήνουμε δύο χωρικά εντοπισμένα, και αρχικώς ανεξάρτητα, qubits να αλληλεπιδράσουν τοπικά με τους χωρικούς βαθμούς ελευθερίας του πεδίου αλλά όχι μεταξύ τους. Η αλληλεπίδραση αυτή διαρκεί σύντομο χρονικό διάστημα, και μετά το πέρας αυτής ποσοτικοποιούμε τον εναγκαλισμό των qubits χρησιμοποιώντας τα εργαλεία του Μέρους II. Βρίσκουμε πως τα δύο qubits είναι εναγκαλισμένα μετά την αλληλεπίδραση, παρότι δεν αλληλεπίδρασαν ποτέ μεταξύ τους, και παρότι μπορούν να απέχουν μέχρι και χωροειδή αποστάση κατά τη διάρκεια της αλληλεπίδρασης. Αυτό που καταφέραμε, είναι να εξάγουμε εναγκαλισμό Σ.Μ. από τον πεδίο και να το μετατρέψουμε σε εναγκαλισμό Δ.Μ. των qubits. Την ποσότητα του τελευταίου τη βρίσκουμε να συμπίπτει ακριβώς με την εύρος της παραβίασης του κριτήριου εναγκαλισμού Σ.Μ. που εφαρμόσαμε στο πεδίο. Τέλος, βρίσκουμε ότι, στη σύντομη αλληλεπίδραση που θεωρήσαμε, ο εναγκαλισμός μπορεί να εξαχθεί από το πεδίο, μόνο αν η θερμοκρασία του πεδίου είναι χαμηλότερη από την κρίσιμη θερμοκρασία και πολύ κοντά στο απόλυτο μηδέν. Επομένως, το φαινόμενο της συμπύκνωσης του πεδίου φαίνεται να ενισχύει την εξαγωγή του εναγκαλισμού.

Λεξεις-Κλειδια: κβαντική, πληροφορία, εναγκαλισμός, πεδίο, εξαγωγή

Contents

Part I

Basic Concepts

Chapter 1

Formalism and measurements

In this chapter, we will introduce the main formalism of quantum theory and the framework of generalized measurements. One of the most important concepts is the (reduced) density matrix, an invaluable tool in the study of entanglement in many body systems which we will encounter in later chapters, so we elaborate on how this concept comes about. We also emphasize on the ambiguity of the ensemble interpretation, since, as we shall see, a single density matrix can in principle describe infinite many different ensembles of quantum systems. This property will be directly related, later on, with the quantum teleportation procedure. Finally, the theory of generalized quantum measurements will be discussed. A very nice introduction in these concepts can be found in [5], [7].

1.1 Schrödinger's equation

Schrödinger's equation is the first thing one learns in an introductory course of quantum mechanics, and we know that it's given by the relation

$$\hat{H}\left|\Psi\left(t\right)\right\rangle = i\hbar\frac{\partial}{\partial t}\left|\Psi\left(t\right)\right\rangle, \tag{1.1}$$

where $\hat{H}$ is the Hamiltonian operator (whose eigenstates have well-defined energy), and $\left|\Psi\left(t\right)\right\rangle$ is the quantum state of the system. We are particularly interested in the time evolution of the state $\left|\Psi\left(t\right)\right\rangle$; i.e. if we know the state of a quantum system at an initial time t_0, how is it going to evolve at later times $t > t_0$? The answer is given by Schrödinger's equation that rules the dynamics of the system, making its evolution deterministic. The solution of (1.1) will give

$$\left|\Psi\left(t\right)\right\rangle = \hat{U}\left(t-t_0\right)\left|\Psi\left(t_0\right)\right\rangle, \tag{1.2}$$

where $\hat{U}\left(t-t_0\right) = \mathrm{T}\left\{\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t}\hat{H}\left(t\right)dt\right]\right\}$. The notation T denotes the time-ordering prescription[1] of the exponential, in the case we expand it in Taylor series. The operator $\hat{U}$ is unitary $\left(\hat{U}^{\dagger}\hat{U}=1\right)$ and consequently the time evolution of the system is known as *unitary evolution*.

At this point let us make some necessary comments. When we use Schrödinger's equation (1.1) for a quantum system, e.g. a harmonic oscillator or the Hydrogen atom,

we have assumed that the quantum system under study is isolated from all other *quantum* systems in the universe. This type of isolated systems are called *closed quantum systems*, and their main characteristic is that they evolve in time via the unitary evolution (1.2).

On the other hand, it's impossible to completely isolate a physical system from its (quantum) environment. In real life, a quantum system is almost always a part of a larger system, interacting with it. This is, for example, the main problem in the actual construction of a reliable quantum computer. A very characteristic example of a quantum system, that is impossible to isolate it from its environment *in principle*, is the hydrogen atom. If the atom was truly isolated, then an excited state should never decay, since the energy eigenstates of the atom are only affected by a phase factor during their time evolution. But, as we all know, an excited atom always decays. Why is that? That's because the charged particles it's made of, always interact with the vacuum state of the electromagnetic field. The vacuum state is present everywhere in spacetime, hence charged particles interact with it no matter where they are. As a result, the system is no longer closed and decays. These kind of systems, that interact with other quantum systems, are known as *open quantum systems*. In contrast to the isolated closed systems, open quantum systems do not obey the unitary evolution of Schrödinger's equation.

1.2 Pure and mixed ensembles

The concept of an *ensemble* is a very important ingredient in the statistical interpretation of quantum mechanics. Consider, for example, a two-level system in the superposition $|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. A measurement of the system in the $\{|0\rangle, |1\rangle\}$ basis will project $|\Psi\rangle$ in one of the states $|0\rangle, |1\rangle$ with probability 50%. However, if we had a single system in our possession, it would not be possible to confirm such a statistical prediction, since the measurement process destroys the initial quantum states, preventing us from repeating it. Thus, we should half a collection of quantum systems identically prepared in the quantum state $|\Psi\rangle$, so that by performing subsequent measurements on all of them, we can check the statistical prediction of the theory. At this point, we would like to point out that the need for an ensemble of systems *does not* imply that a quantum state has a meaning only for ensembles of systems and not for individual particles. The truth is, no one really knows what's the case; the measurement problem and the interpretation of quantum mechanics [10] are still one of the most important open questions in the foundations of science.

There are two kinds of ensembles:

• The *pure* ensembles - or, in other words, pure states - in which a system of the ensemble has a definite pure state $|\Psi\rangle$ which is the same for every single member of the ensemble. An example of a pure ensemble, is a collection of Hydrogen atoms in the ground state $|g\rangle$.

• The *mixed* ensembles - or, mixed states - are composed by sub-ensembles, where each one of them corresponds to some definite pure state $|\Psi_i\rangle$. Such a mixed ensemble will be completely known, if we know the participation rates $p_1, p_2, \ldots, p_N$ of each ensemble. Each p_i is defined as the number of systems N_i in the ensemble i with quantum state $|\Psi_i\rangle$ divided by the number N of systems of the whole ensemble, i.e. $p_i = \frac{N_i}{N}$. In other words,

it's the probability that we find the state $|\Psi_i\rangle$ in the ensemble, and of course it holds that $\sum_i p_i = 1$. An example of such a mixed ensemble is an atomic gas at finite temperature T. This ensemble of atoms will be mixed, containing a percentage $p_i \propto Exp\left[-E_i/k_BT\right]$ of atoms in an energy eigenstate $|E_i\rangle$. Hence, we don't know exactly which atom has which state, we only know the probability that some atom has some state. This kind of ensembles, as it's obvious, cannot be described by pure states and require a more general and fundamental tool, the density matrix. We will introduce the concept of the density matrix in a while. Finally, note that this concept of mixedness is present in classical physics as well, for example in classical statistical mechanics where we work with probabilities and don't know the properties of individual systems.

1.2.1 The difference between mixed states and superposition

Let us examine the following situation. Assume that we have two different ensembles:

• A pure ensemble, the member of which are all described by the pure state

$$|\Psi\rangle = c_1 |\Psi_1\rangle + c_2 |\Psi_2\rangle + \ldots + c_N |\Psi_N\rangle , \tag{1.3}$$

where $|\Psi_i\rangle$ are orthogonal to each other, i.e. $\langle \Psi_j \mid \Psi_i\rangle = \delta_{ij}$, and $p_i = |c_i|^2$ is the probability that $|\Psi\rangle$ will collapse to $|\Psi_i\rangle$ after a measurement. After measuring all the systems of this pure ensemble, a percentage p_i of them will have acquired the state $|\Psi_i\rangle$.

• A mixed ensemble, consisting of a percentage p_1 of systems in the aforementioned state $|\Psi_1\rangle$, p_2 in $|\Psi_2\rangle$, etc.

After measuring the two ensembles, we find that the states $|\Psi_i\rangle$ exist with the same percentage in both ensembles. This fact may confuse someone to consider the two ensembles equivalent regarding the measurement of physical quantities. Here we will show that this is not the case, and draw an important conclusion out of this. Let us calculate the mean value of an arbitrary observable described by the hermitian operator $\hat{A}$, using both ensembles to compare the results. The mixed ensemble give the following mean value,

$$\left\langle \hat{A} \right\rangle_M = \sum_i p_i \left\langle \hat{A} \right\rangle_i = \sum_i p_i \langle \Psi_i | \hat{A} | \Psi_i \rangle , \tag{1.4}$$

while the pure ensemble,

$$\begin{aligned} \left\langle \hat{A} \right\rangle_P = \langle \Psi | \hat{A} | \Psi \rangle &= \sum_i |c_i|^2 \langle \Psi_i | \hat{A} | \Psi_i \rangle + \sum_{i \neq j} p_i p_j \langle \Psi_i | \hat{A} | \Psi_j \rangle \\ &= \left\langle \hat{A} \right\rangle_M + \underbrace{\sum_{i \neq j} p_i p_j \langle \Psi_i | \hat{A} | \Psi_j \rangle}_{\text{interference terms}} . \end{aligned} \tag{1.5}$$

The difference between the two ensembles is obvious. The superposition of states in (1.4) is not just ignorance, as in the mixed ensemble, but the superposed states can interfere with each other giving rise to the so-called interference terms. So, we conclude that a

superposition of pure states is fundamentally different from a simple statistical mixture of pure states. The superposition principle, inherent in the formalism of quantum theory, has many implications in many practical and fundamental issues which we will examine in *Part II* when we'll talk about quantum entanglement. Now, it's time that we introduce the *density matrix*.

1.3 Density matrix

In our previous analysis, we saw that a mixed ensemble cannot be described by just one pure state, while a pure ensemble, of course, can. The density matrix is a useful tool that can describe any kind of ensemble, fully describing it. Moreover, it can also describe the aforementioned open quantum systems, and not only the closed -isolated- ones, making it of invaluable importance. In the next chapters of this thesis, we are going to exploit this tool to study quantum entanglement. So, let's examine it thoroughly.

1.3.1 Definition of density matrix

The density matrix gives a full description of an ensemble of quantum systems. If it was known to us, for example, we would be able to calculate the mean value of any observable with respect to this ensemble. Let us calculate the mean value of an arbitrary observable $\hat{A}$ and see how the density matrix comes about.

Assume that we have a mixed ensemble of quantum states, a p_1 percentage of which is described by the quantum state $|\Psi_1\rangle$, a p_2 percentage by $|\Psi_2\rangle$ etc. What the mean value $\left\langle \hat{A} \right\rangle$ would be in such an ensemble? From general statistics, we know that it will be equal to the weighted average value of the quantum mechanical mean values that correspond to the pure states of the ensemble. For example, the observable $\hat{A}$ has a mean value $\langle \Psi_i | \hat{A} | \Psi_i \rangle$ with respect to the pure state $|\Psi_i\rangle$, but the latter pure state exists in a percentage p_i in the whole ensemble, making its total contribution to the mean value $\left\langle \hat{A} \right\rangle$ to be $p_i \langle \Psi_i | \hat{A} | \Psi_i \rangle$. By making the same arguments for every i, we find that final mean value $\left\langle \hat{A} \right\rangle$ to be,

$$\left\langle \hat{A} \right\rangle = \sum_i p_i \langle \Psi_i | \hat{A} | \Psi_1 \rangle . \tag{1.6}$$

We can end up to the same formula (1.6) having as a starting point the relation

$$\left\langle \hat{A} \right\rangle = \sum_n P_n \, a_n, \tag{1.7}$$

where a_n are the eigenvalues of $\hat{A}$, i.e. $\hat{A} |a_n\rangle = a_n |a_n\rangle$, and P_n are the probabilities of their appearance in the mixed ensemble under study. Let us think, what the mathematical expression for P_n would be. Suppose that we measure $\hat{A}$, projecting each of the $|\Psi_i\rangle$ of the ensemble in some eigenvector $|a_n\rangle$ of $\hat{A}$. The appearance of the eigenvalue a_n presupposes the retraction of $|\Psi_i\rangle$ out of the ensemble -having a probability of retraction p_i- and, afterwards, the appearance of a_n from a measurement of $|\Psi_i\rangle$, having a probability of appearance $P_{i,n} = |\langle n \mid \Psi_i \rangle|^2$. The joint probability for both to happen is the just the

product $p_i P_{i,n}$. Consequently, the total probability of appearance of the eigenvalue a_n from *any* pure state of the ensemble, is the sum of each joint probability over all i,

$$P_n = \sum_i p_i P_{i,n} = \sum_i p_i |\langle n \mid \Psi_i \rangle|^2. \tag{1.8}$$

Based on the expression (1.8), the mean value (1.7) becomes,

$$\left\langle \hat{A} \right\rangle = \sum_n P_n \, a_n = \sum_{i,n} p_i |\langle n \mid \Psi_i \rangle|^2 a_n. \tag{1.9}$$

We would like to write this expression quite differently. Our purpose is to distinguish all those parameters that solely characterize the ensemble (e.g. p_i, $|\Psi_i\rangle$), from those that concern the arbitrary observable $\hat{A}$ that we want to measure (e.g. $a_n, |n\rangle$). The former quantities, that characterize the ensemble and not the observable, we give us the wanted expression for the density matrix. Due to,

$$|\langle n \mid \Psi_i \rangle|^2 = \langle n \mid \Psi_i \rangle \langle n \mid \Psi_i \rangle^* = \langle n \mid \Psi_i \rangle \langle \Psi_i \mid n \rangle , \tag{1.10}$$

and

$$|n\rangle \, a_n = \hat{A} \, |a_n\rangle , \tag{1.11}$$

the expression (1.9) will take the desired form,

$$\begin{aligned} \left\langle \hat{A} \right\rangle &= \sum_{i,n} p_i \langle n \mid \Psi_i \rangle \langle \Psi_i | \, \hat{A} \, |n\rangle \\ &= \sum_n \langle n | \underbrace{\left(\sum_i p_i \, |\Psi_i\rangle \langle \Psi_i| \right)}_{\hat{\rho}} \hat{A} \, |n\rangle = \sum_n \langle n | \hat{\rho} \hat{A} \, |n\rangle \\ &= Tr \left[\hat{\rho} \hat{A} \right] , \end{aligned} \tag{1.12}$$

where we defined the density matrix to be

$$\hat{\rho} = \sum_i p_i \, |\Psi_i\rangle \langle \Psi_i| \, . \tag{1.13}$$

The trace in (1.12) is defined as sum over the diagonal elements of the operator $\hat{\rho}\hat{A}$ in some arbitrary basis. The value of the trace of a matrix does not depend on a specific choice of basis, since it's invariant under unitary transformations of quantum states. Notice that the density matrix involves quantities that characterize the ensemble, and not the observable. Knowledge of the density matrix allows to calculate the mean value of any observable on the ensemble. The expression (1.13) of $\hat{\rho}$ can also describe pure ensembles, for which all the systems are described by a single state, by setting $p_i = 1, \; p_{j \neq i} = 0$,

$$\hat{\rho} = |\Psi_i\rangle \langle \Psi_i| \, . \tag{1.14}$$

As a final statement, let us mention that the expectation value (1.12) expressed via some operator $\hat{\rho}$ (the density matrix) is more general that is seems to be. While investigating the existence of possible new axioms for quantum theory, Gleason[2] found that under very general assumptions, the average value of a projection operator $\hat{P}$ is given by

$$\left\langle \hat{P} \right\rangle = Tr \left(\hat{\rho} \hat{P} \right) ,$$

where $\hat{\rho}$ is a non-negative operator with unit trace (we'll see about that in the next section), which depends solely on the preparation of the quantum system and not on the choice of the projector P (just as we said). So, the density matrix turns out to be most fundamental, since the axioms of quantum theory *require* it, and we are not using it just for convenience. For more information on Gleason's theorem, besides the original paper, see [8].

1.3.2 Properties

At this point, we will prove various important properties of the density matrix. To be more general we will work with a mixed density matrix, since the pure state is a sub-case of the mixed one.

• If we evaluate the trace (1.13) of the density matrix using some arbitrary basis $\{|n\rangle\}$, we will find

$$\begin{aligned} Tr\hat{\rho} &= \sum_n \langle n|\,\hat{\rho}\,|n\rangle = \sum_i p_i \langle \Psi_i| \left(\sum_n |n\rangle\langle n|\right)|\Psi_i\rangle \\ &= \sum_i p_i = 1. \end{aligned} \tag{1.15}$$

So, the trace of any density matrix will always be unity if the states $\{|\Psi_i\rangle\}$ are also normalized to unity.

• Next, we will prove a criterion that can distinguish if a given density matrix is mixed or pure. Let us calculate $Tr\hat{\rho}^2$ for an arbitrary ensemble,

$$\begin{aligned} Tr\hat{\rho}^2 &= Tr\left[\left(\sum_i p_i\,|\Psi_i\rangle\langle\Psi_i|\right)\left(\sum_j p_j\,|\Psi_j\rangle\langle\Psi_j|\right)\right] \\ &= Tr\left[\sum_{i,j} p_i p_j \langle\Psi_i \mid \Psi_j\rangle\,|\Psi_i\rangle\langle\Psi_j|\right] \\ &= \sum_{i,j} p_i p_j |\langle\Psi_i \mid \Psi_j\rangle|^2, \end{aligned} \tag{1.16}$$

and due to Schwartz's inequality ,

$$|\langle\Psi_i \mid \Psi_j\rangle| \leq \||\Psi_i\rangle\| \cdot \||\Psi_j\rangle\| = 1, \tag{1.17}$$

we finally have

$$Tr\hat{\rho}^2 \leq 1. \tag{1.18}$$

It's easy to see that for any pure state, the equality is satisfied,

$$Tr\hat{\rho}^2_{pure} = 1, \tag{1.19}$$

while for a general mixed state it's strictly lower than one,

$$Tr\hat{\rho}^2_{mixed} < 1. \tag{1.20}$$

The quantity $Tr\hat{\rho}^2$ is known as the *purity* of the state, and will be really useful and indispensable to our work later on. Other important properties of the density matrix that are straightforward to prove from its definition, are

1. $\hat{\rho}$ is a hermitian operator: $\hat{\rho} = \hat{\rho}^\dagger$
2. $\hat{\rho}$ is a positive semidefinite operator, i.e. $\forall\, |\Psi\rangle$ it always holds that $\langle\Psi|\,\hat{\rho}\,|\Psi\rangle \geq 0$,
3. $Tr\hat{\rho} = 1$ - Normalization, probabilities sum to one..

1.3.3 The reduced density matrix

In this thesis, we are going to study the dynamics of quantum systems that interact with an environment (other quantum systems). However, we will not be able to access (via measurements) the Hilbert space of the environment, only the quantum system under study is accessible. So, the next question is of extreme importance in our study; can the statistical predictions on this subsystem be described without making any reference to the environment? The answer is positive, and is given by the concept of the *reduced density matrix*.

For simplicity, consider two particles, whose joint Hilbert space is $H_A \otimes H_B$, described by the state $|\Psi\rangle_{AB}$. If $\{|i_A\rangle\}$ is an orthonormal basis of H_A and $\{|\mu_B\rangle\}$ an orthonormal basis of H_B, then $\{|i_A\rangle \otimes |\mu_B\rangle\}$ is an orthonormal basis for $H_A \otimes H_B$. Hence, the state $|\Psi\rangle$ can be expressed as,

$$|\Psi\rangle_{AB} = \sum_{i,\mu} a_{i,\mu}\,|i_A\rangle \otimes |\mu_B\rangle\,, \tag{1.21}$$

where $\sum\limits_{i,\mu} |a_{i,\mu}|^2 = 1$.

As we said, we care of measuring observables of only one of the subsystems, say A. Consider the other system B as the "environment" of A. Measuring an observable of A means that this observable belongs to the Hilbert space H_A of particle A. A general observable of this kind, has the form

$$\hat{M}_A \otimes \hat{1}_B, \tag{1.22}$$

where the unity that acts on H_B denotes that no projection takes place on that space. Our purpose now is to calculate the expectation value of this observable, and bring the formula in a form similar to (1.12), but now our goal is to form a density matrix that includes only elements of system A. This will be the so-called reduced density matrix of system A. Let's see,

$$\begin{aligned}
\left\langle \hat{M}_A \right\rangle &= {}_{AB}\langle\Psi|\,\hat{M}_A \otimes \hat{1}_B|\Psi\rangle_{AB} \\
&= \sum_{j,\nu} a^*_{j,\nu}\,({}_A\langle j| \otimes {}_B\langle\nu|)\,\hat{M}_A \otimes \hat{1}_B \sum_{i,\mu} a_{i,\mu}\,(|i\rangle_{\mathrm{A}} \otimes |\mu\rangle_{\mathrm{B}}) \\
&= \sum_{i,j,\mu} a^*_{j,\mu} a_{i,\mu A}\,\langle j|\,\hat{M}_A\,|i\rangle_A \\
&= Tr\left[\hat{M}_A \hat{\rho}_A\right],
\end{aligned} \tag{1.23}$$

where we defined the reduced density matrix

$$\hat{\rho}_A = Tr_B \left(|\Psi\rangle_{AB\,AB} \langle\Psi| \right) = \sum_{i,j,\mu} a^*_{j,\mu} a_{i,\mu} |i\rangle_{A\,A} \langle j| \,, \tag{1.24}$$

involving quantities that characterize solely the particle A, not B. The notation of the partial trace Tr_B means that the sum on the diagonal elements is taken only with respect to states belonging to Hilbert space H_B. In a sense, we "integrate-out" the degrees of freedom that we don't have access to, and physically this means that for every possible configuration of system A the effect of system B on it (due to the coupling) is averaged over all possible configurations of B. As a result of this averaging procedure, quantum correlations that are encoded between the two systems A and B are lost. These correlations, as we will see in the next part, can be so strong that seem to challenge basic, long-standing and accepted premises about the principles of nature. See Section 2.3 for a discussion on this. Finally, the reduced density matrix is a legitimate density matrix, hence can be shown to satisfy the three aforementioned properties of hermiticity and positivity.

1.3.4 Ambiguity of the ensemble interpretation

In this section we will report on a very important feature of the density matrix, and specifically its *unitary freedom* which is summarized in the following statement

A given density matrix can describe infinitely many ensembles prepared in different ways.

Let us elaborate a little on what we mean by "preparing ensembles". Consider, for example, the following mixed density matrix, describing particles of spin-$\frac{1}{2}$,

$$\begin{aligned} \hat{\rho} &= \frac{1}{2} |\uparrow_z\rangle \langle\uparrow_z| + \frac{1}{2} |\downarrow_z\rangle \langle\downarrow_z| \\ &= \frac{1}{2} |\uparrow_x\rangle \langle\uparrow_x| + \frac{1}{2} |\downarrow_x\rangle \langle\downarrow_x| \end{aligned} \tag{1.25}$$

We can see that two different ensembles are described by the same density matrix. The first ensemble, is constituted by 50% particles with spin-up in the z-direction and 50% with spin-down in the z-direction, while the second ensemble, is similar but with spins pointing to the x-direction. Experimentally, the preparing procedures of each of these two ensembles are totally different, and yet the statistical predictions of each are identical. We would like to explore this characteristic in a more general framework.

Consider the following density matrix,

$$\hat{\rho} = \sum_i \left| \tilde{\Psi}_i \right\rangle \left\langle \tilde{\Psi}_i \right| , \tag{1.26}$$

where the states $\left\{ \left| \tilde{\Psi}_i \right\rangle \right\}$ are not normalized; $\left| \tilde{\Psi}_i \right\rangle = \sqrt{p_i} \, |\Psi_i\rangle$, with $|\Psi_i\rangle$ now being normalized. Let us relate the states $\left| \tilde{\Psi}_i \right\rangle$ with some other states $\left| \tilde{\Phi}_i \right\rangle$ via an unknown -for now- transformation,

$$\left| \tilde{\Psi}_i \right\rangle = \sum_j u_{ij} \left| \tilde{\Phi}_i \right\rangle. \tag{1.27}$$

We want to find a condition that the transformation u_{ij} should satisfy, so that the density matrix (1.26) that describes the $\left\{\left|\tilde{\Psi}_i\right\rangle\right\}$ ensemble can also describe the $\left\{\left|\tilde{\Phi}_i\right\rangle\right\}$ ensemble,

$$\begin{aligned}\hat{\rho} &= \sum_i \left|\tilde{\Psi}_i\right\rangle\left\langle\tilde{\Psi}_i\right| = \sum_{i,j,k} u_{ij}u_{ik}^* \left|\tilde{\Phi}_j\right\rangle\left\langle\tilde{\Phi}_k\right| = \sum_{j,k}\left(\sum_i u_{ki}^\dagger u_{ij}\right)\left|\tilde{\Phi}_j\right\rangle\left\langle\tilde{\Phi}_k\right| \\ &== \sum_j \left|\tilde{\Phi}_j\right\rangle\left\langle\tilde{\Phi}_k\right|,\end{aligned} \tag{1.28}$$

where the last "double" equality denotes that we demand the equality to be true. What condition shall u_{ij} satisfy? It's easily seen that the matrix u_{ij} has to be unitary in order for the desired equality to be true, i.e.

$$\sum_i u_{ki}^\dagger u_{ij} = \delta_{kj} \quad \Leftrightarrow \quad U^\dagger \cdot U = 1. \tag{1.29}$$

Writing the above in matrix forms, considering

$$\left|\tilde{\Psi}\right\rangle = \begin{pmatrix} \left|\tilde{\Psi}_1\right\rangle \\ \left|\tilde{\Psi}_2\right\rangle \\ \vdots \end{pmatrix}, \quad \text{and} \quad \left|\tilde{\Phi}\right\rangle = \begin{pmatrix} \left|\tilde{\Phi}_1\right\rangle \\ \left|\tilde{\Phi}_2\right\rangle \\ \vdots \end{pmatrix}, \tag{1.30}$$

then the quantum states of each ensemble is connected to the other via a unitary transformation,

$$\left|\tilde{\Psi}\right\rangle = U\left|\tilde{\Phi}\right\rangle, \quad \text{with} \quad U^\dagger \cdot U = 1. \tag{1.31}$$

Since there are infinitely many unitary matrices, the density matrix describes infinitely many ensembles,

$$\begin{aligned}\hat{\rho} &= \sum_i \left|\tilde{\Psi}_i\right\rangle\left\langle\tilde{\Psi}_i\right| = \sum_j \left|\tilde{\Phi}_j\right\rangle\left\langle\tilde{\Phi}_k\right| \\ &= \sum_j p_i \left|\Psi_i\right\rangle\left\langle\Psi_i\right| = \sum_j q_i \left|\Phi_i\right\rangle\left\langle\Phi_i\right|.\end{aligned} \tag{1.32}$$

This property of the density matrix plays a crucial role in quantum teleportation, as discussed in Section 2.4. In the same context, of great importance is the so-called *GHJW theorem* which states that in the case of two entangled systems, there is always an observable to be measured on one of the systems so that *any* ensemble can be realised in the other system. See [7] for a nice treatment.

1.3.5 Eigenvectors and eigenvalues of a density matrix

Consider an arbitrary mixed state,

$$\hat{\rho} = \sum_j p_i \left|\Psi_i\right\rangle\left\langle\Psi_i\right|. \tag{1.33}$$

In general, the states $\{|\Psi_i\rangle\}$ are not orthogonal to each other, but in the case that they are it holds,

$$\hat{\rho}\,|\Psi_i\rangle = p_i\,|\Psi_i\rangle\,. \tag{1.34}$$

What this means, is that eigenvalue p_i corresponds to the probability of $|\Psi_i\rangle$'s existence in the ensemble. We see that eigenvalues of a density matrix are probabilities, and probabilities need to sum to one; hence we can now understand why we demand this specific normalization $Tr\hat{\rho} = \sum_i p_i = 1$. The ensemble comprised from $\hat{\rho}$'s eigenvectors is only one out of infinite possible ensembles that can be described by this density matrix, as we explicitly proved in the previous section. However, it's the only ensemble consisting only of orthogonal states.

1.4 Generalized measurements

In the usual textbook treatment of measurement theory, only the orthogonal -so called "von Neumann"- measurements are being presented, and constitute one of the axioms of quantum mechanics. That's natural, since a measurement of a spin we will either show up or down, we always have a definite answer, and that's the concept of orthogonal measurements. Mathematically, these measurements collapse the initial quantum state $|\Psi\rangle$, onto some state out a possible set of possible orthogonal states. These measurements are described by a set of orthogonal projection operators $\{E_a\}$,

$$\text{i) } \hat{E}_a = \hat{E}_a^\dagger, \quad \text{ii) } \hat{E}_a\hat{E}_b = \hat{E}_b\delta_{ab}, \quad \text{iii) } \sum_a \hat{E}_a = 1. \tag{1.35}$$

The probability that the result of a measurement, onto some state $\hat{\rho}$, is "a" , is

$$p\,(a) = Tr\left(\hat{\rho}\hat{E}_a\right), \tag{1.36}$$

while the new density matrix *after* the measurement (the "collapsed" one) will be,

$$\hat{\rho}' \to \frac{\hat{E}_a\hat{\rho}\hat{E}_a}{Tr\left(\hat{\rho}\hat{E}_a\right)} \quad \text{- if we know that the measurement result is } a \tag{1.37}$$

$$\to \sum_a \hat{E}_a\hat{\rho}\hat{E}_a \quad \text{- if don't know what the measurement result is.} \tag{1.38}$$

Here we encounter for the first time the close connection between a mixed density matrix and ignorance of the observer. As you can see, we can assign to the same quantum system two different density matrices, a pure one (if the observer knows the result), or a mixed one if the observer doesn't know the specific result of the measurement but knows the probability distribution for each result to come about, and averages over all of them.

Example .

Let's work out a specific example. Suppose that a two-dimensional quantum system is in the pure state $|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ (or $\hat{\rho} = |\Psi\rangle\langle\Psi|$ in the density matrix formalism),

hence the vectors $\{|0\rangle, |1\rangle\}$ constitute a basis. Say that we want to make a measurement on that basis (e.g. these vectors are the eigenvectors of an observable). According to the above analysis, we define the projection operators

$$\hat{E}_0 = |0\rangle\langle 0|, \quad \text{and} \quad \hat{E}_1 = |1\rangle\langle 1|, \tag{1.39}$$

that satisfy the above requirements, e.g.

$$\sum_i \hat{E}_i = |0\rangle\langle 0| + |1\rangle\langle 1| = 1.$$

Using (1.36), the probability that the outcome "0" will come about, is

$$\begin{aligned} p(0) &= Tr\left(|\Psi\rangle\langle\Psi|\hat{E}_0\right) = \langle\Psi|\hat{E}_0|\Psi\rangle \\ &= |\langle 0 \mid \Psi\rangle|^2 = \frac{1}{2}, \end{aligned} \tag{1.40}$$

which is just Born's rule for the probability formula, while the density matrix after the measurement will be,

$$\hat{\rho}' \to \frac{\hat{E}_0\hat{\rho}\hat{E}_0}{Tr\left(\hat{\rho}\hat{E}_0\right)} = |0\rangle\langle 0|, \tag{1.41}$$

as expected. But what if we don't know the measurement outcome? Or, what the density matrix would be if we measured an ensemble of systems in this basis, but don't know what the state of its single system is? (These are equivalent questions) It follows from (1.38) that,

$$\begin{aligned} \hat{\rho}' \to \sum_a \hat{E}_a\hat{\rho}\hat{E}_a &= |\langle 0 \mid \Psi\rangle|^2 |0\rangle\langle 0| + |\langle 1 \mid \Psi\rangle|^2 |1\rangle\langle 1| \\ &= \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|, \end{aligned} \tag{1.42}$$

hence, as expected, half of the systems will be in $|0\rangle\langle 0|$ and the other half in $|1\rangle\langle 1|$. However, as we shall see in the next section, these kind of measurements -the orthogonal von Neumann measurements- are very restrictive, and they actually belong to a much larger set of possible measurements that can be performed on a quantum system.

1.4.1 Operator-Sum representation and POVM

Suppose you have a particle, whose wavefunction $\psi(x)$ is spread in space, and you want to make a position measurement. Ideally, a real position measurement collapses the wavefunction to single position $|x\rangle$. However this is unrealistic. First of all, from the mathematical point of view, a perfectly orthogonal measurement that distinguishes a single position would lead to an infinite spread in momentum $\Delta p = \infty$, which means that a moment later the particle would be far away. But this is not what we observe in a bubble chamber, is it? Why do particles follow straight lines if they have $\Delta p = \infty$ in all directions? The answer, is that even the particles in a bubble chamber are not so localized and have some finite Δx. Even the bubble chamber does not localize the

particle completely, the measurement is not so accurate in this sense. In general, maybe we do want our measurements not to be so accurate. For example, if you want to validate that a particle is inside the room, you don't have to localize it in a mathematical point! A localization with a spread much smaller than the volume you want to find it in is good enough. Other reasons for wanting to perform such "inaccurate" measurements, is that maybe we want to observe a quantum state without interrupting it very much, since an orthogonal measurements completely destroys the initial state. But what kind of measurement is this if it's not of the orthogonal von-Neumann type? In this section we will describe how to perform such measurements.

We will axiomatically accept that von Neumann measurements are possible; That's natural, since a measurement of a spin in a Stern-Gerlach experiment will either show spin-up or spin-down. In order to perform a non-orthogonal measurement on a quantum state, we will another quantum state known as *ancilla* on which the orthogonal measurements will be performed. Assume that our -to be measured- quantum state is $|\varphi\rangle_{\mathrm{A}}$, while the ancillary system is initially in some state $|0\rangle_{\mathrm{B}}$. The two systems are initially uncorrelated, which means that their joint quantum state is,

$$|\varphi\rangle_A \otimes |0\rangle_B. \tag{1.43}$$

Now we will drive the joint system via some unitary transformation U_{AB}, which could be an interaction between the systems A and B, and the choice of U depends on what we want to do on sytem A. The joint state will evolve to

$$\begin{aligned}
\hat{U}_{AB}\left(|\varphi\rangle_A \otimes |0\rangle_B\right) &= \sum_{\mu,\nu} |\mu\rangle_B {}_B\langle\mu|\, \hat{U}_{AB}|\nu\rangle_B\, |\varphi\rangle_A {}_{\mathrm{B}}\langle\nu \mid 0\rangle_{\mathrm{B}} \\
&= \sum_{\mu} \underbrace{{}_B\langle\mu|\, \hat{U}_{AB}|0\rangle_B}_{\hat{M}_\mu} |\varphi\rangle_A \otimes |\mu\rangle_B \\
&= \sum_{\mu} \hat{M}_\mu |\varphi\rangle_A \otimes |\mu\rangle_B.
\end{aligned} \tag{1.44}$$

The operators $\hat{M}_\mu = {}_B\langle\mu|\, \hat{U}_{AB}|0\rangle_B$ act only on the Hilbert space H_A, and when act on the initial state $|\varphi\rangle_A$ they alter it in a desirable way if we suitable engineer the desired interaction $\hat{U}_{AB}$ and suitable choose the observable to measure on the ancilla (i.e. choose proper basis $\{|\mu\rangle_B\}$). When we orthogonally measure the ancilla B on the basis $\{|\mu\rangle_B\}$, the state of system A will collapse to one the states $\left\{\hat{M}_\mu|\varphi\rangle_A\right\}$ (where the index μ is counting the states). It's easy to see that these states are not orthogonal to each other, i.e.

$${}_{\mathrm{A}}\langle\varphi|\, \hat{M}^\dagger_{\mu'}\, \hat{M}_\mu|\varphi\rangle_A \neq \ \delta_{\mu',\mu}, \tag{1.45}$$

since the measurement operators are not orthogonal like the von Neumann ones, i.e.

$$\hat{M}^2_\mu \neq \hat{M}_\mu, \tag{1.46}$$

hence, the states after the collapse overlap.

We want to generalize our formalism, so consider the case where the initial state of system A is a mixed state $\hat{\rho}_A = \sum_i p_i|\varphi_i\rangle_{AA}\langle\varphi_i|$, and the initial state of joint system $A+B$ is

$$\hat{\rho}_A \otimes |0\rangle_{BB}\langle 0|\,. \tag{1.47}$$

After applying the joint unitary operator $\hat{U}_{AB}$, the reduced state of the system A after this interaction will be,

$$\begin{aligned}\$\left[\hat{\rho}_A\right] &= Tr_B\left[\hat{U}_{AB}\left(\hat{\rho}_A \otimes |0\rangle_{BB}\langle 0|\right)\hat{U}_{AB}^{\dagger}\right] \\ &= \sum_{\mu} {}_B\langle\mu|\,\hat{U}_{AB}|0\rangle_B \hat{\rho}_{AB}\,\langle 0|\,\hat{U}_{AB}|\mu\rangle_B \\ &= \sum_{\mu} \hat{M}_{\mu}\hat{\rho}_A\hat{M}_{\mu}^{\dagger}.\end{aligned} \tag{1.48}$$

This is the evolved reduced density matrix of our desired system expressed in the *operator-sum representation* (see [5], [7]). The symbol \$ acting on the initial $\hat{\rho}_A$ is known as a *superoperator*, and gives the evolved reduced density matrix after an interaction has taken place (or, a transformation in general). The evolved state $\$\left[\hat{\rho}_A\right]$ can be easily seen to satisfy the usual density matrix criteria,

- $Tr_A\$\left[\hat{\rho}_A\right] = 1 \;\text{ since }\; \sum_{\mu}\hat{M}_{\mu}^{\dagger}\hat{M}_{\mu} = 1,$ (1.49)
- $\$[\hat{\rho}_A]^{\dagger} = \$\left[\hat{\rho}_A\right]$ (1.50)
- $\$\left[\hat{\rho}_A\right] \geq 0.$ (1.51)

The operator-sum representation of the reduced matrix is, ofcourse, not unique, since for a given $\hat{U}_{AB}$ one may choose to measure a different observable in the ancilla B, thus preparing a different (but statistically equivalent) ensemble in A. Thus we face, once more, the ambiguity of the ensemble interpretation discussed in Section 1.3.4 and its connection to the *GHJW* theorem. For example, in (1.48) we could perform the partial trace on B using another basis $\{|\nu\rangle_B\}$ instead of $\{|\mu\rangle_B\}$,

$$\begin{aligned}\$\left[\hat{\rho}_A\right] &= Tr_B\left[\hat{U}_{AB}\left(\hat{\rho}_A \otimes |0\rangle_{BB}\langle 0|\right)\hat{U}_{AB}^{\dagger}\right] \\ &= \sum_{\nu} {}_B\langle\nu|\,\hat{U}_{AB}|0\rangle_B \hat{\rho}_{AB}\,\langle 0|\,\hat{U}_{AB}|\nu\rangle_B \\ &= \sum_{\nu} \hat{N}_{\nu}\hat{\rho}_A\hat{N}_{\nu}^{\dagger},\end{aligned} \tag{1.52}$$

where the new operators $\left\{\hat{N}_{\nu}\right\}$ are related to $\left\{\hat{M}_{\mu}\right\}$ via

$$\begin{aligned}\hat{N}_{\nu} = {}_B\langle\nu|\,\hat{U}_{AB}|0\rangle_B &= \sum_{\mu} {}_B\langle\nu \mid \mu\rangle_{BB}\langle\mu|\,\hat{U}_{AB}|0\rangle_B \\ &= \sum_{\mu} {}_B\langle\nu \mid \mu\rangle_B \hat{M}_{\mu},\end{aligned} \tag{1.53}$$

which is actually equivalent to (1.31).

What we have achieved is to present a formulation and an operational way to perform non-orthogonal measurements on quantum systems, with the use of an ancilla, orthogonal measurements on the ancilla and global unitary transformation of the joint system.

The measurements on the ancilla induce a non-orthogonal measurement on our quantum system of interest. The latter measurements may not be orthogonal to each other, like the von Neumann ones, but they still have a measurement outcome, say "μ". In the von Neumann case, every outcome μ was associated with a projective operator $\hat{E}_\mu$, and the probability of getting that outcome after a measurement was given by (1.36),

$$p(\mu) = Tr\left(\hat{\rho}\hat{E}_\mu\right). \tag{1.54}$$

We want to do the same thing with the generalized measurements, i.e. to associate a measurement outcome with an operator, just like what we did with von Neumann measurements, $\mu \leftrightarrow \hat{E}_\mu$. Suppose that the initial state of the quantum system of interest is a general mixed state,

$$\hat{\rho}_A = \sum_i p_i |\varphi_i\rangle_{AA} \langle\varphi_i|, \tag{1.55}$$

and we perform on this state a non-orthogonal measurement via the above procedure; i.e. couple the system A with a system B, evolve them jointly via some unitary $\hat{U}_{AB}$ and measure orthogonally some observable on the ancilla. The result of this procedure, is our desired non-orthogonal measurement that corresponds to some operators $\left\{\hat{M}_\mu\right\}$ (see (1.48)), giving us the final reduced density matrix of A,

$$\$\left[\hat{\rho}_A\right] = \sum_\mu \hat{M}_\mu \hat{\rho}_A \hat{M}_\mu^\dagger, \tag{1.56}$$

where the density matrices $\hat{M}_\mu \hat{\rho}_A \hat{M}_\mu^\dagger$ are not normalized, i.e. $Tr\left[\hat{M}_\mu \hat{\rho}_A \hat{M}_\mu^\dagger\right] \neq 1$. So, in order to see with what probability each density matrix $\hat{M}_\mu \hat{\rho}_A \hat{M}_\mu^\dagger$ occurs in the mixture $\$\left[\hat{\rho}_A\right]$, we have to normalize them,

$$\hat{M}_\mu \hat{\rho}_A \hat{M}_\mu^\dagger \rightarrow \frac{\hat{M}_\mu \hat{\rho}_A \hat{M}_\mu^\dagger}{Tr_A\left[\hat{M}_\mu^\dagger \hat{M}_\mu \hat{\rho}_A\right]} \equiv \hat{\rho}'_\mu, \tag{1.57}$$

since $Tr\hat{\rho}'_\mu = 1$. Now the evolved density matrix can be written in its regular mixed form where the probabilities can be recognized,

$$\begin{aligned} \$\left[\hat{\rho}_A\right] &= \sum_\mu \hat{M}_\mu \hat{\rho}_A \hat{M}_\mu^\dagger = \sum_\mu \underbrace{Tr_A\left[\hat{M}_\mu^\dagger \hat{M}_\mu \hat{\rho}_A\right]}_{p(\mu)} \hat{\rho}'_\mu \\ &= \sum_\mu p(\mu)\, \hat{\rho}'_\mu, \end{aligned} \tag{1.58}$$

and the probability formula for the outcome μ is,

$$p(\mu) = Tr_A\left[\hat{M}_\mu^\dagger \hat{M}_\mu \hat{\rho}_A\right]. \tag{1.59}$$

We conclude, that, after a non-orthogonal measurement on a quantum system, the initial state $\hat{\rho}_A$ collapses to a statistical ensemble of states $\left\{\hat{\rho}'_\mu\right\}$, each appearing with probability

$p(\mu)$. From the probability formula (1.59), it's obvious that we can associate the measurement outcome μ with the hermitian operator $\hat{M}_\mu^\dagger \hat{M}_\mu$ just as we wanted. The set of all these operators $\left\{\hat{M}_\mu^\dagger \hat{M}_\mu\right\}$, for every measurement outcome μ, is generally known as a *POVM* (Positive operator valued measure). So, every time we perform a non-orthogonal -not so accurate- measurement, we say that we perform a *POVM*, described by some measurement operators $\left\{\hat{F}_\mu \equiv \hat{M}_\mu^\dagger \hat{M}_\mu\right\}$ that satisfy the following properties,

$$\text{i) } \hat{F}_\mu^\dagger = \hat{F}_\mu, \quad \text{ii) } \hat{F}_\mu \geq 0, \quad \text{iii) } \sum_\mu \hat{F}_\mu = 1, \quad \text{iv) } \hat{F}_\mu^2 \neq \hat{F}_\mu. \tag{1.60}$$

The main characteristic of a POVM is the property (iv), i.e. they are not projection operators. For a complete treatment of POVMs and superoperators, see [5].

As a final remark, we would like to make a connection of what we presented here with the main subject of this work, which is entanglement. All these generalized measurements, we saw that, they are possible if we couple the quantum system of interest with another quantum system. This coupling leads to entanglement between the two systems, which we will define later on. Previously, we mentioned that by choosing a different observable to measure on the ancilla (the other quantum system), we actually prepare a different state in our quantum system. But, the time at which we make this measurement on the ancilla, the two systems may be well-separated by each other, and need not interact during that time. How is it possible, then, that a measurement on one alters the state of the (well separated) other? These mind-blowing effects of quantum mechanics are employed in the field of quantum information and computing[5] to perform actual real life tasks, that classical physics would never allow. See *Part* II for an analysis.

Part II

Discrete-Variable Entanglement

Chapter 2

Bipartite Entanglement

Entanglement can exist between arbitrarily many particles, and it's known as multipartite entanglement. However, in this introductory part we will thoroughly study bipartite entanglement, i.e. entanglement between two particles, or two independent degrees of freedom in general. We do that for two reasons; the bipartite case is the most well-studied, in contrast to the multipartite one, and also it is the simplest, making all the concepts easier to grasp. All the necessary mathematical formalism is reviewed in the Appendix, and we refer the reader there in case needed. For a review on discrete-variable entanglement theory see [3], [4]. Useful references on Quantum Information theory, that include a careful analysis of these concepts, are [5]-[7].

2.1 Entanglement of pure states

Suppose that we have two quantum systems A and B, belonging to the (independent) Hilbert spaces H_A and H_B respectively, and described by the pure quantum state $|\psi\rangle_{AB} \in H_A \otimes H_B$. For example, this state could describe the spin degrees of freedom of two particles. We say that $|\psi\rangle_{AB}$ is *entangled* if it cannot be written in the product form

$$|\psi\rangle_{AB} \neq |\varphi\rangle_A \otimes |\chi\rangle_B, \tag{2.1}$$

where $|\varphi\rangle_A \in H_A$ and $|\chi\rangle_B \in H_B$. Otherwise, it's called *separable*.

But what is so special about entangled states that cannot be written in the form (2.1)? Let us think classically for a moment. Suppose that Alice, living in New York, has in her possession a spin-$\frac{1}{2}$ particle in the superposition $|\varphi\rangle_A = \frac{1}{\sqrt{2}}(|\uparrow_z\rangle_A + |\downarrow_z\rangle_A)$. Her particle is locked in her volt (which actually is a vacuum chamber), well isolated and not able to interact with anything else, and only Alice can perform spin-measurements on it whenever she wants to. Moreover, her friend Bob, who lives in Athens (far away from New York), has another spin-$\frac{1}{2}$ particle in a different superposition, $|\chi\rangle_B = \frac{1}{\sqrt{2}}|\uparrow_z\rangle_B + \sqrt{\frac{3}{2}}|\downarrow_z\rangle_B$, locked in his own volt. As is obvious, Alice's particle and Bob's particle, separated by thousands of kilometres, are totally independent with each other and uncorrelated. Now let us see how the statistics of measurements behave under the when both Alice and Bob measure the spins of their particles. If they measure in the $\left\{|s_z\rangle_{A,B}\right\}$ basis, with $s = \uparrow, \downarrow$, the probability that Alice finds the result s is $|{}_A\langle s_z \mid \varphi\rangle_A|^2$, while the probability that

Bob finds s' is $|{}_B\langle s'_z \mid \chi\rangle_B|^2$. Now let us ask, what is the probability that Alice finds s *and* Bob finds s'? From the theory of probabilities we know that when two events are independent, the probability of a joint event is the product of probabilities of the individuals. So, following the previous notation, the corresponding probability is

$$|{}_A\langle s \mid \varphi\rangle_A|^2 \cdot |{}_B\langle s' \mid \chi\rangle_B|^2 \tag{2.2}$$

The only quantum state of the joint system A *and* B that gives these statistics is

$$|\psi\rangle_{AB} = |\varphi\rangle_A \otimes |\chi\rangle_B, \tag{2.3}$$

and that is why this state is called *separable*, since it describes independent degrees of freedom.

However, in the quantum domain there are pure quantum states that describe jointly two independent systems, like the two isolated spin-$\frac{1}{2}$ particles above, but cannot be written in this separable form (2.1). These are the so-called entangled states, and one example of such a state is

$$\left|\psi^-\right\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle_A|\downarrow_z\rangle_B - |\downarrow_z\rangle_A|\uparrow_z\rangle_B\right). \tag{2.4}$$

Again, this state could describe the spin degrees of freedom of Alice's and Bob's isolated particles, even though they are, otherwise, independent from each other. What is so weird about this state is that, even though it describes two independent particles, the measurement statistics that this state induces is different from a product of probabilities, even though these particles may be separated by arbitrarily large distance. This non-product form has significant consequences. Each particle cannot be described separately of the other particle, i.e. particle A cannot be described by a quantum state that doesn't involve particle B. Moreover, particle A (and B) doesn't have a specified spin direction prior to measurement as can be seen by the superposition in (2.4). But a measurement, by either Alice or Bob, on the isolated particle will automatically determine the spin direction of the other particle. For example, if Alice makes a measurement on her spin and finds the up direction, the whole quantum state of the joint system will have collapsed in

$$\left|\psi^-\right\rangle_{AB} \to |\uparrow_z\rangle_A|\downarrow_z\rangle_B, \tag{2.5}$$

which automatically determines that Bob's particle has its spin downwards. A lot of reasonable questions arise:

• *There seems to be an "action at a distance"*[9] *induced by Alice's measurement of her own spins on Bob's particles, by instantly determining the spin direction of his particles. Does this mean that we can send information faster than light?*

Think of the following scenario. Alice and Bob, separated by an arbitrarily large distance, share 100 entangled pairs of spin-$\frac{1}{2}$ particles, all in the quantum state (2.4). Alice wants to send a message to Bob by taking advantage of the entanglement. By measuring the spin of her own particles, she can instantly determine the spin direction of Bob's particles due to the entanglement. Then Bob can measure the spin components of his own particles, and consequently read the message which was instantly send by Alice's

measurement (a cryptographic method could be used by properly assigning letters to the series of spins, e.g. $A = \uparrow\uparrow\uparrow$, $B = \downarrow\downarrow\downarrow$, $C = \uparrow\downarrow\downarrow$, etc.). Entanglement seems to be able to violate causality in that way, because -remember- Alice and Bob are separated by a spacelike distance, which means that the order of events may differ from one observer to the other. For example, in Alice's reference frame, it's she that first sends the message and *then* Bob reads it. But in another boosted reference frame that moves relative to Alice's, it's Bob that first reads the message and *then* Alice sends it thus violating causality. Thankfully, what saves the principle of causality and forbids the possibility of sending information faster than light is the *randomness* of the measurement process. Alice cannot determine beforehand the spin direction that her spins will acquire after her measurement, hence she is not able to deterministically control the measurement process and send a message. After Alice's measurement, Bob will still observe just a random "meaningless" sequence of up and down spins. Mathematically, all the statistics of Bob's local measurements on his own spins are described by the reduced density matrix $\hat{\rho}_B$, occurring after tracing over the degrees of freedom of Alice's particles, i.e.

$$\begin{aligned} \hat{\rho}_B &= Tr_A \left[\left| \psi^- \right\rangle_{AB} \left\langle \psi^- \right| \right] \\ &= \frac{1}{2} |\uparrow\rangle_B \langle\uparrow| + \frac{1}{2} |\downarrow\rangle_B \langle\downarrow| \\ &= \frac{1}{2} \hat{1}. \end{aligned} \tag{2.6}$$

This is a maximally mixed state (in the sense that all outcomes are equiprobable), since it's proportional to the unit operator, and completely independent of Alice's measurements on her spins.

This simple example provides a strong argument towards the true intrinsic randomness of quantum theory. If this randomness was not intrinsic, and we could find a way to somehow determine beforehand the results of quantum measurements, then quantum entanglement would be able to violate the deep principle of causality.

• *The argumentation given above, that a measurement of a state here instantly determines the quantum state there, is not very convincing. Perhaps Alice's and Bob's spins have a well determined direction before the measurement and Alice and Bob are just ignorant of it!*

This is a first thought almost everyone encounters when first learn about this phenomenon. Imagine the following "classical" situation: Two electrons come out of a physical process where angular momentum is conserved and consequently their spins are *always* anti-correlated and also given by $|\psi^-\rangle_{AB}$, i.e. when one is spin-up the other is spin-down and vice versa, with probability $\frac{1}{2}$. A rational thought is that these electrons do have a definite spin-direction prior to measurement, but we just cannot know if electron "A" is spin up and electron "B" is spin down or vice versa, due to our incomplete knowledge of the physical situation that produced the electrons. The measurement we perform afterwards only unveils the *pre-existing* spin direction of the particles. This intuition, heritage of classical physics and generally known as *local realism*, will turn out to be incorrect! In the next chapter we will talk about the infamous Bell's inequalities which proved that

nature is not both local and realistic. We will save the discussion for this latter chapter.

A very useful tool for determining whether a given bipartite pure quantum state is entangled, is the so-called Schmidt decomposition given by the following Lemma.

Lemma 1. *(Schmidt decomposition)*
Let a bipartite system AB be in a pure state $|\psi\rangle = \sum_{i,j=1}^{d_A,d_B} c_{ij} |a_i\rangle \otimes |b_j\rangle \in H_\mathrm{A} \otimes H_B$*, where* d_A*,* d_B *are the dimensions of the Hilbert spaces* H_A *and* H_B *respectively. There exists an orthonormal basis* $\{|\alpha_i\rangle\}$ *of* H_A *and* $\{|\beta_j\rangle\}$ *such that* $|\psi\rangle$ *can be expressed in the form*

$$|\psi\rangle = \sum_{m=1}^{R} \lambda_m |\alpha_m\rangle \otimes |\beta_m\rangle , \tag{2.7}$$

where λ_m *are real coefficients and* $R \leq \min\{d_A, d_B\}$ *is the so-called Schmidt rank (or number). The* λ_m *are uniquely determined by the eigenvalues of the matrix* $CC^\dagger$*, where* $C = (c_{ij})$ *is the matrix formed by the coefficients in Eq. (2.7). If* $R > 1$ *then the state is entangled.*

The proof of this useful result is not difficult and can be found in [5]. The Schmidt decomposition gives a clear definition of what it means for a bipartite pure state to be entangled, and an operational way of how to find if a given pure state is entangled. In the case of mixed states, as we will see, the situation is not so clear.

An important property of the Schmidt number is that it *cannot be increased* by any local unitary transformations, of the form $U_A \otimes U_B$, on the particles. What this means is that a unitary transformation of the state of each particle separately (not collective transformations) cannot generate entanglement. A separable state, like $|\uparrow\rangle_A \otimes |\uparrow\rangle_B$, which has a Schmidt number $R = 1$, cannot get entangled by a local transformation of the form

$$|\uparrow\rangle_A \otimes |\uparrow\rangle_B \rightarrow \hat{U}_A|\uparrow\rangle_A \otimes \hat{U}_B|\uparrow\rangle_B,$$

since the Schmidt number cannot increase. In order to generate an entangled state with $R > 1$, e.g.

$$\frac{1}{\sqrt{2}} \left(|\uparrow\rangle_A \otimes |\uparrow\rangle_B + |\downarrow\rangle_A \otimes |\downarrow\rangle_B\right),$$

and consequently entangle to qubits, we must bring them together and allow them to interact. The interaction will implement a collective transformation $U_{AB} \neq U_A \otimes U_B$ which can increase the Schmidt number, thus generating entanglement between the particles.

2.2 Entanglement of mixed states

Suppose now that a bipartite system is described by a mixed quantum state, ρ_{AB}, where we follow the conventional nomenclature A=Alice and B=Bob. The most general form of a mixed state is

$$\hat{\rho}_{AB} = \sum_i p_i |\varphi_i\rangle_{AB} \langle\varphi_i|, \tag{2.8}$$

with $\sum_i p_i = 1, \quad Tr\hat{\rho}_{AB}^2 < 1$, and $|\varphi_i\rangle_{AB} \in H_A \otimes H_B$. The purity being less than 1, denotes that their some uncertainty on which quantum state, $|\varphi_i\rangle_{AB}$, was prepared having a statistical mixture.

For convenience, once more, assume that this state describes the spin degrees of freedom of two spatially separated spin-$\frac{1}{2}$ particles, with one being kept by Alice and the other by Bob. In order for a density matrix of the form (2.8) to be separable, it should be possible, for Alice and Bob, to produce it locally via Local Operations and Classical Communication ($LOCC$), and also the statistics should follow the product rule that we discussed in the previous section.

Definition 1. *A, generally mixed, density matrix $\hat{\rho}_{AB}$ is called separable (or classically correlated) if it can be expressed as a sum of product states, i.e.*

$$\hat{\rho}_{AB} = \sum_i p_i \hat{\rho}_{A,i} \otimes \hat{\rho}_{B,i}, \tag{2.9}$$

Otherwise, it's called entangled.

We can see that a general separable state is just a statistical mixture of product (hence, separable) states $\hat{\rho}_{A,i} \otimes \hat{\rho}_{B,i}$, where $\hat{\rho}_{A,i},\ \hat{\rho}_{B,i}$ could be either mixed or pure. This mixture is statistical and not coherent, meaning that the different states do not interfere with each other as is the case in a superposed state. It's easy to see how to create such a state, (2.9), locally via LOCC. Suppose that Alice and Bob share a random number generator, and for every outcome i of the generator they have agreed to produce the state $\hat{\rho}_{A,i} \otimes \hat{\rho}_{B,i}$ locally. They can program the generator in such a way so that it produces the outcome i with probability p_i, and via telephone they communicate the result to each other. Having done that with many quantum systems, they have managed to prepare an ensemble systems AB where each pair is described by $\hat{\rho}_{AB} = \sum_i p_i \hat{\rho}_{A,i} \otimes \hat{\rho}_{B,i}$. It's obvious, now, that Alice's particle A, described by $\hat{\rho}_{A,i}$ is correlated in a classical way with Bob's particle described by $\hat{\rho}_{B,i}$. The word *classical* denotes the classical mechanism that was used to prepare this state, i.e. local operations and classical communication. It's useful to understand this, since an entangled state involves correlations, between the particles A and B, that cannot be described by a classical model as the above (2.9).

2.3 The violation of Bell's inequalities

Quantum mechanics is as strange as it gets. It seems that quantum correlations, namely the entanglement, can violate causality but it does not. Remember that we are working with non-relativistic quantum mechanics at this point, so we wouldn't expect causality to be respected. The weird thing is that quantum correlations do respect it. Moreover, as Einstein objected (see EPR paradox), entanglement seems to influence two space-like separated quantum systems, and that was a feature of Quantum theory that he didn't like, even if causality was not at stake. Entanglement defies a physical requirement that is obvious in our classical world, namely that of *local realism*. This nomenclature has a simple meaning: All objects have definite properties prior to measurement (*reality*), while these properties cannot be influenced in any way by experiments performed in regions that are space-like separated from the object (*locality*).

2.3.1 The EPR paradox

Einstein disliked Quantum Theory for, at least, two reasons; its intrinsic randomness and quantum entanglement. Particularly, he used the property of entanglement in his famous paper [9], together with B. Podolsky and N. Rosen, to show that *"the quantum-mechanical description of physical reality given by the wave functions is not complete"*, citing their words. Their original argument was based on entanglement between the spatial wavefunctions of the particles. We will change it a little bit, and use entanglement between the spin degrees of freedom for simplicity. The conclusions are going to be the same.

The argument goes like this; Consider two particles in the singlet state,

$$\left|\psi^{-}\right\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle_A|\downarrow_z\rangle_B - |\downarrow_z\rangle_A|\uparrow_z\rangle_B\right), \tag{2.10}$$

following the Alice and Bob example. Alice is in possession of particle A while Bob of particle B. They are both separated by an arbitrarily large distance, so the particles cannot interact in any way. Now, suppose that Alice measures the observable $\hat{\sigma}_{z,A} \otimes \hat{1}_B$, i.e. her particle's spin the z-direction. There are two possible ways for the quantum state to collapse,

$$\textit{Measurement of } \hat{\sigma}_{z,A} \otimes \hat{1}_B$$

$$\left|\psi^{-}\right\rangle_{AB} \to |\uparrow_z\rangle_A|\downarrow_z\rangle_B, \quad \text{with 50 \% probability} \tag{2.11}$$

$$\left|\psi^{-}\right\rangle_{AB} \to |\downarrow_z\rangle_A|\uparrow_z\rangle_B, \quad \text{with 50 \% probability.} \tag{2.12}$$

As you can see, Bob's particle will acquire a spin $|\downarrow_z\rangle_B$ or $|\uparrow_z\rangle_B$, but surely it will have a definite z-direction. Now, go back. Suppose that Alice decides to measure her particle not in the z-direction, $\hat{\sigma}_{z,A} \otimes \hat{1}$, but in the x-direction, i.e. $\hat{\sigma}_{x,A} \otimes \hat{1}$. Remember that the observables $\hat{\sigma}_{x,A},\ \hat{\sigma}_{z,A}$ do not commute. Let us see what would happen in that case,

$$\textit{Measurement of } \hat{\sigma}_{x,A} \otimes \hat{1}_B$$

$$\left|\psi^{-}\right\rangle_{AB} \to |\uparrow_x\rangle_A|\downarrow_x\rangle_B, \quad \text{with 50 \% probability} \tag{2.13}$$

$$\left|\psi^{-}\right\rangle_{AB} \to |\downarrow_x\rangle_A|\uparrow_x\rangle_B, \quad \text{with 50 \% probability,} \tag{2.14}$$

where we used the relations

$$|\uparrow_z\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_x\rangle + |\downarrow_x\rangle\right), \quad |\downarrow_z\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_x\rangle - |\downarrow_x\rangle\right). \tag{2.15}$$

If this measurement is performed, Bob's particle will acquire a definite spin in the x-direction, and not in the z-direction as the previous measurement as before. The states $|\downarrow_z\rangle_B, |\uparrow_z\rangle_B$ are totally different from $|\downarrow_x\rangle_B, |\uparrow_x\rangle_B$, and Alice's choice of what observable to measure entirely influences Bob's particle!

But EPR didn't arrive at this conclusion. Instead, they thought that two space-like separated and non-interacting particles cannot influence one another, and the reality of Bob's particle cannot depend on Alice's choice of measurement ($\hat{\sigma}_{z,A}$ or $\hat{\sigma}_{x,A}$). So, they argued that, we can assign to Bob's particle two different wave functions, $|\uparrow, \downarrow_z\rangle_B$ or

$|\uparrow, \downarrow_x\rangle_B$. They concluded that the wave function is not an element of the physical reality of the system under investigation, since the above assignment was arbitrary, and quantum theory is incomplete; An underlying local, realistic and deterministic theory was thought to exist.

A hundred years after the discovery of Quantum Mechanics, and there is still no consensus on what its formalism actually mean [10]. Due to the difficulty of understanding what this theory actually *is*, i.e. how to interpret its formalism, a new line of research was initiated by John Bell[11], in order to find out what this theory is *not*. In the next section we will analyse Bell's inequalities and show that Einstein's notion of *local realism* is defied by the experiments.

2.3.2 A generalized Bell's inequality: The *CHSH* inequality

Most of us, including the EPR trio, want to believe that nature is local and realistic. Perhaps, such a theory, that satisfies our classical prejudices, underlies quantum mechanics. Perhaps, nature is deterministic and quantum randomness is just an illusion, objects may have properties irrespectively of whether we measure them, and two space-like separated objects cannot interact in any way. The list goes on, and anyone can think of anything, but how can we be sure if any of this premises is respected by nature? John Bell was the first to show, in [11], that the concept of *local realism* can, actually, be tested via quantitative criteria.

What is important to understand, is that Bell's criteria are not a property of quantum mechanics, they are not based on quantum theory, they actually do not depend on any underlying theory. They are just criteria that should be satisfied by *any* local realistic theory of any type, no matter how complicated. Bell realised that the statistics of the measurements made by two space-like separated observers on their systems, are quantitatively bounded if we demand locality, i.e. independence of the observable Alice chooses to measure on her particle to the observable that Bob chooses to measure on his particle, and reality, i.e. both particles have definite properties independent of whether we measure them or not (although unknown to us in general). Now let us see how to formulate local realism, our proof will not depend on any theory as you will see.

An experimental setup to check local realism

Imagine the experimental situation depicted in Figure 2.1, a source emits two photons in opposite directions, each going through a polariser and eventually detected with either a horizontal $(-)$ or vertical $(+)$ polarisation. Before we continue, let us note that "photons" are only just a particular realisation of a possible experiment to check local realism, in general it could anything, e.g. electrons, atoms, etc. Also, we used the word "polarisation"; we shouldn't. This word refers to some physical quantity, and since we don't know anything about the underlying theory (if it's not quantum mechanics), we should not refer to physical terms. And that's the power of Bell's theorem, it doesn't depend on the underlying physics, but only on the measurement outcomes.

So, we rephrase: What is important in the experiment is that, after the two photons have gone through a device called polariser (with which they interacted in an unknown way), they will eventually hit either the up-detector +1 or the down-detector -1, as seen in Figure 2.1. Every time a photon hits a detector we hear a click and we note the

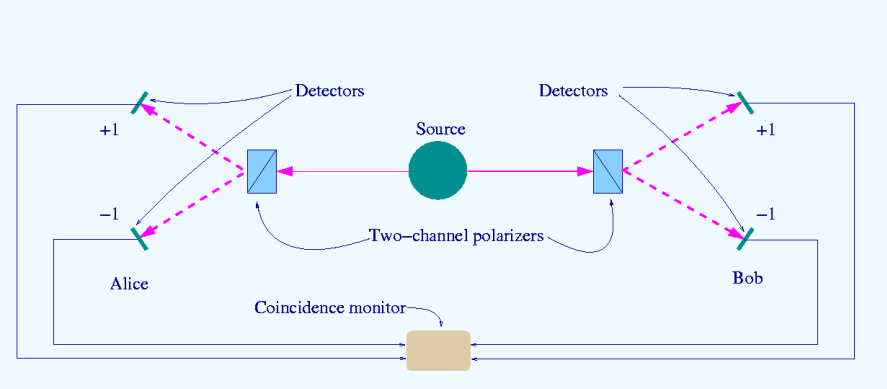

Figure 2.1: **Scheme of a "two-channel" Bell test** The source S produces pairs of "photons", sent in opposite directions. Each photon encounters a two-channel polariser whose orientation (a or b) can be set by the experimenter. Emerging signals from each channel are detected and coincidences of four types (++, –, +b•" and b•"+) counted by the coincidence monitor. (From *http://en.wikipedia.org/wiki/Bell's_theorem)*

outcome as +1 or -1 depending on which detector it hit. The two polarisers in each side are identical, and we can change this device's orientation in order to measure different properties of the photon. Since we are unaware of the underlying theory, we can only say that by changing the orientation of the polariser, we manage to change the way it interacts with the photon, and, hence, change the probability by which each detector is hit (i.e. whether the photon will go up or down; this can be checked experimentally). This orientation of the polariser is described by an angle θ, and Alice (controlling the detector on the left) and Bob (controlling the detector on the right) can change that angle at will. When the two polarisers in each side are oriented at the same angle, they have exactly the same properties, they are identical.

The source emits one pair of photons at a time, and the two photons hit Alice's detector (left) and Bob's detector (right) simultaneously. Since the only outcomes are +1 or -1, for each pair of photons there are four possible outcomes,

$$(+1,+1)\,,\quad (-1,+1)\,,\quad (+1,-1)\,,\quad (-1,-1)\,. \tag{2.16}$$

In total, assume that the source emits N photon pairs, with N being large enough so that our statistics are sufficient and statistical errors may be neglected.

Observables & Assumptions

The use of the word observable here, has nothing to do with the observables of quantum theory (hermitian operators etc). Remember that our analysis, at this point, is independent of any theory. What we mean by "observable" at this point is the result of the measurement +1 or -1, which depends on the angle of the polariser θ. So, perhaps, the nomenclature "measurement outcome" would be preferable instead of "observable".

So, Alice's measurement outcome, to be called A, is going to depend on the angle θ_A of her polariser, namely $A_j(\theta_A)$, and Alice is allowed to choose the angle θ_A freely before the detection of her particle. Same for Bob, $B_j(\theta_B)$. As we previously mentioned, the only possible values for the observables are two,

$$A_j(\theta_A) = \pm 1, \;\; B_j(\theta_B) = \pm 1, \tag{2.17}$$

where j denotes the particular photon pair. Notice that we make no demand for the outcome $A_j(\theta_A)$, of Alice's detector, to depend on the angle θ_B of Bob's detector, and this is an implication of **locality**. The behaviour of Alice's photon cannot depend on the angle, θ_B, that Bob is going to choose for his detector, which, by the way, is space-like separated from Alice's. This is our first crucial, and perhaps obvious for most, assumption.

In each run of our experiment, where a single photon pair is emitted, we will allow Alice and Bob to choose the angle of their polarisers freely, out of a set of two angles for each, i.e.

$$\theta_A \in \{a_1, a_2\}\,, \quad \theta_B \in \{b_1, b_2\}\,. \tag{2.18}$$

So, Alice(Bob) is free to choose the angle $\theta_A(\theta_B)$ to be either $a_1(b_1)$ or $a_2(b_2)$ in each run. The angles a_i, b_i, that comprise the set (2.18) of the possible angles, must be the *same* in each run of the experiment.

Consequently, every photon pair j is described by four numbers that denote the outcomes of the possible experiments, i.e.

$$A_j\,(a_1)\,,\; A_j\,(a_2) \;\; - \;\; \text{For Alice's photon} \tag{2.19}$$

$$B_j\,(b_1)\,,\; B_j\,(b_2) \;\; - \;\; \text{For Bob's photon.} \tag{2.20}$$

Here, $A_j\,(a_i)$ represents the measurement outcome for the photon j, if Alice chose the angle of her polariser to be a_i, and correspondingly for Bob. But keep in my mind, that in each run of the experiment, we do only one measurement on each photon of the pair. So, if Alice chooses to measure $A_j\,(a_1)$ then $A_j\,(a_2)$ will be left unmeasured. However, the experiment $A_j\,(a_2)$ *could* have been performed, and if it was, there would be a particular measurement outcome, $A_j\,(a_2) = \pm 1$. We don't know what that outcome would be, if it would be either $+1$ or -1, but we assume that it would be something. In other words, we assume that unperformed experiments on a photon have results[13], although unknown.

This is the second crucial assumption of our analysis, where the first was that of locality, and is generally known as the assumption of **reality**. Reality, in this case, means that properties of a particle exist prior to measurement, that a measurement simply unveils the already existing unknown property and doesn't create that property. So, it seems to be legitimate to talk about measurement outcomes of unperformed experiments. Note that in the classical world we do this all the time, and this assumption is also as "obvious" as the one of locality. These two assumptions combined is what is known as *local realism*.

Now let us move on to the next step, to the formation of the inequality.

The *CHSH* inequality

In the previous paragraph, we attached in Alice's photon the properties $A_j\,(a_1)\,,\; A_j\,(a_2)$, i.e. the possible measurement outcomes if these measurements were performed, and correspondingly to Bob' photon, $B_j\,(b_1)\,,\; B_j\,(b_2)$. These two photons belong to the same photon pair j that was emitted from the Source depicted in Figure 2.1. We define the following quantity for the photon pair j,

$$S_j = A_j\,(a_1)\,B_j\,(b_1) + A_j\,(a_1)\,B_j\,(b_2) + A_j\,(a_2)\,B_j\,(b_1) - A_j\,(a_2)\,B_j\,(b_2)\,. \tag{2.21}$$

It can be easily verified that

$$S_j = \pm 2, \tag{2.22}$$

for every combinations of values,

$$A_j(a_1) = \pm 1, \;\; A_j(a_2) = \pm 1, \;\; B_j(b_1) = \pm 1, \;\; B_j(b_2) = \pm 1, \tag{2.23}$$

of the possible measurement outcomes. In order to see this just re-arrange the terms in (2.21) as

$$S_j = A_j(a_1)\left(B_j(b_1) + B_j(b_2)\right) + A_j(a_2)\left(B_j(b_1) - B_j(b_2)\right). \tag{2.24}$$

Try all the different combinations (2.23), and you will see that you will always get $S_j = \pm 2$.

So, whatever angle Alice and Bob chooses to make the measurement, whatever the result of that measurement is, and whatever the result of the unperformed experiments would be, the value of S_j will *always* be ± 2. This fact is a consequence of our two assumptions, that nature is local and realistic, and remember that we are only referring to measurement outcomes performed on space-like separated systems, and make no mention on the possible underlying theory!

Assume that we perform this experiment N times, meaning that the source has emitted a total of N photon pairs. For each photon pair j, with $j \in [1, N]$, we form the quantity S_j, (6.1). Now, we form the mean value of this quantity over all the photon pairs,

$$\langle S \rangle = \frac{1}{N} \sum_{j=1}^{N} S_j, \tag{2.25}$$

and since $S_j = \pm 2, \; \forall j$, it holds that

$$-2 \leq \langle S \rangle \leq +2. \tag{2.26}$$

This is a Bell inequality, known as the *CHSH inequality* [12]. The original inequality of John Bell [11] is a special case of this, more general, inequality. If nature is local and realistic, this inequality should *always* be respected, by any physical system.

2.3.3 A home experiment with coins

Up to this point, we have made no reference to quantum theory. The objects that we are allowed to use, and measure various properties of them, in order to verify/falsify the Bell inequality (2.26) can be arbitrary. In the previous analysis we used photons, and some measuring instruments called polarisers in order to measure different properties of the photons, since these are mostly used in experiments. However, the words "photon" and "polarisers" are not intuitive concepts for anyone. Here we propose a home experiment, that can be performed by anyone, using just two coins.

The two coins will substitute the photons and the polarisers will be substituted by our own eyes, which will "measure" (or simply, unveil) different properties of the coins. Imagine the experimental setup as in Figure 2.1, but the source now will emit, not photons but, a pair of coins in each run; one coin towards Alice and one coin towards Bob. The

detectors in each side (that could be the eyes of Alice and Bob) measure some property of the coins. Each coin is assumed to have four properties that can be measured, say a_1, a_2, b_1 and b_2, and each property can take two possible values, ± 1, just like in (2.23). Say that Alice chooses to measure one of the properties a_1 and a_2 in each run of the experiment, where the possible outcomes of these measurements are

$$A_j(a_1) = \pm 1, \quad A_j(a_2) = \pm 1, \tag{2.27}$$

with a_1 denoting the *material* property of a coin, i.e.

$$\begin{aligned} A_j(a_1) &= +1 : \text{The coin is Gold} \\ A_j(a_1) &= -1 : \text{The coin is Copper,} \end{aligned}$$

and a_2 denoting the *texture*, i.e.

$$\begin{aligned} A_j(a_2) &= +1 : \text{The coin is Shiny} \\ A_j(a_2) &= -1 : \text{The coin is Dull.} \end{aligned}$$

One the other hand, Bob will choose to measure one of the properties b_1 or b_2,

$$B_j(b_1) = \pm 1, \quad B_j(b_2) = \pm 1, \tag{2.28}$$

with b_1 denoting the *size* of a coin, i.e.

$$\begin{aligned} B_j(b_1) &= +1 : \text{The coin is Large} \\ B_j(b_1) &= -1 : \text{The coin is Small,} \end{aligned}$$

and b_2 denoting the *currency*, i.e.

$$\begin{aligned} B_j(b_2) &= +1 : \text{The coin is Euro} \\ B_j(b_2) &= -1 : \text{The coin is Dollar.} \end{aligned}$$

Index j denotes the j^{th} pair of coins emitted by the Source, and the measurements on each pairs of coins always satisfy

$$\begin{aligned} S_j &= A_j\left(a_1\right) B_j\left(b_1\right) + A_j\left(a_1\right) B_j\left(b_2\right) + A_j\left(a_2\right) B_j\left(b_1\right) - A_j\left(a_2\right) B_j\left(b_2\right) \\ &= \pm 2, \end{aligned} \tag{2.29}$$

for every possible combination of measurements, just like in our discussion in Section 2.3.2. Just from this fact we expect the CHSH inequality always to hold for the coins. But let us elaborate a little on the measuring procedure. Since the coins are classical objects, and their properties are always visible, Alice and Bob can measure all the properties of each coin just by looking at it. But, in order to simulate the experimental conditions using quantum systems (e.g. photons), where we cannot measure all the properties of a photon at once, assume that Alice and Bob can measure only *one* property of a coin in each run. So, in each run only one of the following joint observables is actually measured,

$$A_j\left(a_1\right) B_j\left(b_1\right), \quad A_j\left(a_1\right) B_j\left(b_2\right), \quad A_j\left(a_2\right) B_j\left(b_1\right), \quad A_j\left(a_2\right) B_j\left(b_2\right), \tag{2.30}$$

and the rest are left unmeasured. What this means is that S_j is ..unobservable! Then how are we going to test the CHSH inequality?

We will use the following line of reasoning. Say that the Source emits N pairs of coins in total, and assume that we have measurements of the observable $A_j(a_1) B_j(b_1)$ for every single pair of coins. If we had such a list of measurements of this observable, for all the coins, then the mean value of this observable would be

$$\langle A(a_1) B(b_1) \rangle = \frac{1}{N} \sum_{j=1}^{N} A_j(a_1) B_j(b_1). \tag{2.31}$$

However, such a list of measurements is not possible in all cases, for various reasons. For example, if Alice and Bob choose to measure another observable, then $A_j(a_1) B_j(b_1)$ will be left unmeasured. The system that is being measured may either be destroyed by the measurement or affected in a way that changes all its properties, so we are forced to do only one measurement on the system under consideration. So, the actual mean value (2.31) in an experiment of such kind, will not contain all the measured values $j \in [1, N]$, but only some of them, depending on how many (and which) times, of the total N runs of the experiment, Alice and Bob chose to measure this particular observable. Suppose that they measured it M times out of the total N, with $M < N$. If M and N are large enough numbers, and the measurements have been subtracted randomly, then it approximately holds that

$$\frac{1}{M} \sum_{i=1}^{M} A_i(a_1) B_i(b_1) \approx \frac{1}{N} \sum_{j=1}^{N} A_j(a_1) B_j(b_1) = \langle A(a_1) B(b_1) \rangle, \tag{2.32}$$

where, to avoid confusion in the notation, $A_{i=1}(a_1)$ is not necessarily the same to $A_{j=1}(a_1)$.

So, the experimentally accessible measurements are enough to assure that the mean value will be equal to what it should be, if *all* measurements were accessible. But is the random subtraction truly *random*? Since Alice and Bob do not know the properties of the coins before they make their choice on what property to measure, this process should be random. Even if they do know the properties beforehand, the process will still be random if Alice and Bob have not agreed on what observable to jointly measure. However if they cheat, somehow, by knowing the properties of the coins before they make their choice and they have agreed, beforehand, what observable to jointly measure, they can violate Bell's inequality since (2.32) will no longer hold. It's like throwing a die and knowing, beforehand, what number is going to end up to; If it's going to be 5 you decide not to throw it this time, and, that way, you can exclude all $5s$ from your throws, which is unnatural and is due to cheating. The important thing here is that, (2.32) holds only for random processes. The same reasoning applies to the rest of the observables (2.30). We conclude that,

$$\begin{aligned} \langle S \rangle \approx \frac{1}{M_1} \sum_{i=1}^{M_1} A_i(a_1) B_i(b_1) + \frac{1}{M_2} \sum_{k=1}^{M_2} A_k(a_1) B_k(b_2) + \\ + \frac{1}{M_3} \sum_{l=1}^{M_3} A_l(a_2) B_l(b_1) - \frac{1}{M_4} \sum_{m=1}^{M_4} A_m(a_2) B_m(b_2), \end{aligned} \tag{2.33}$$

where we used different indexes to denote different coin/photon pairs, and the value of the numbers M_i depend on number of times Alice and Bob chose to measure the particular observable. Since the total runs of the experiment are N, it should hold that

$$M_1 + M_2 + M_3 + M_4 = N. \tag{2.34}$$

We would like to point out that, if the expression (2.25) was experimentally applicable, instead of (2.33), then even cheating would not be enough to violate the CHSH inequality! A violation, in that case, would only occur if our assumption of local realism did not hold. However, (2.25) is not applicable in general, so we have to rely on (2.33) and be careful on how to perform the experiment so that the equality between the two quantities will hold.

Equation (2.33) is the formula that is used in the experiments testing Bell's inequality. If we actually do the proposed experiment using coins or any classical object, or just simulate the procedure with an algorithm, we would see no violation of Bell's inequality, no matter what initial correlations between the coins the Source chooses. It is useful to do this at least once, in order to convince oneself, that, it really *couldn't be otherwise.* Yet, it can. Quantum objects, if prepared in a suitable initial entangled quantum state, can violate Bell's inequality as we will see in the next section.

Concluding, we presented a very simple proof of Bell's inequalities and the implications of local realism, without explicitly referring to hidden variables, keeping the proof as simple as possible. Another beautiful and intuitive derivation of Bell's inequalities, where there is no use of concepts like probabilities and hidden variables, can be found in [16]

2.3.4 Experimental violation of Bell's inequality

The first experimental demonstration was that of Freedman and Clauser [14], in 1972, where they used the linear polarization of photons as the "+" and "-" measurements, and found a violation of the CHSH inequality (2.26). Ten years later, the famous experiment of A. Aspect *et. al.* [15] took place with the improvement that they changed the angle of the two polarisers while the photons where in flight. They observed a violation of (2.26) by 5 standard deviations. The following years many experiments confirmed these results, highlighting that of Zeilinger *et. al.* [17], where they observe a violation of CHSH inequality over 30 standard deviations and under strict Einstein locality conditions using photons as well, while experiments have also been conducted, recently, using entangled trapped ions [18] and superconducting Josephson phase qubits [19], instead of photons, increasing even more the accuracy of the violation. A typical experimental curve is depicted in Figure 2.2, where the limits imposed from local realism are undeniably violated. Note that the experimental curve coincides exactly (within experimental error) with the quantum mechanical prediction.

Let us mention, briefly, that in all the aforementioned experimental setups there are certain problems with the experimental design, widely known as *loopholes.* These loopholes can, in principle, be taken advantage of to violate the CHSH inequality even if nature is local and realistic. Examples of such loopholes are detection efficiency, fair sampling, communication or locality, free choice of detector orientations and others. To

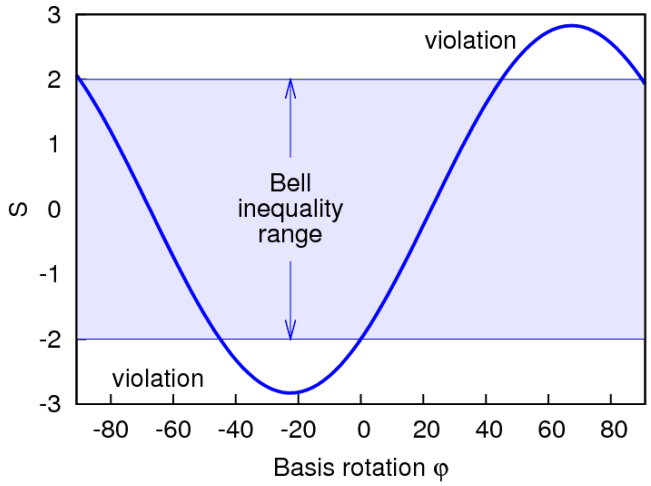

Figure 2.2: **A singlet state violating the CHSH inequality** The range of possible values for the CHSH quantity $\langle S \rangle$ is illustrated and should be respected if nature were local and realistic. The solid curve represent both the experimental findings and the quantum mechanical prediction, for a singlet quantum state. The angle ϕ represents the relative orientation of the two polarisers, i.e. $\phi = a_1 - b_1 = a_2 - b_2$. We see a clear violation of the Bell inequality for some angles. (From *http://www.qolah.org/outreach/x2010.html)*

date, each loophole has been closed in some Bell-type experiment but no test has simultaneously closed all loopholes. Some authors, like E. Santos [20], argue that it is nature that forbids us from closing simultaneously all loopholes, and local realism still holds. The majority of physicists, however, believe that Bell's inequalities will still be violated even if all loopholes are closed (experiments are continuously being proposed to that direction).

2.3.5 The quantum mechanical prediction

Up to this point, we made no reference to an underlying theory in order to derive Bell's inequality, we only assumed nature to be local and realistic. But we have a very good candidate for this underlying theory, i.e. quantum mechanics! We would like to express the following mean value (2.33),

$$\langle S \rangle \approx \frac{1}{M_1} \sum_{i=1}^{M_1} A_i(a_1) B_i(b_1) + \frac{1}{M_2} \sum_{k=1}^{M_2} A_k(a_1) B_k(b_2) + \\ + \frac{1}{M_3} \sum_{l=1}^{M_3} A_l(a_2) B_l(b_1) - \frac{1}{M_4} \sum_{m=1}^{M_4} A_m(a_2) B_m(b_2),$$

in the quantum mechanical language, and see what this theory predicts when we do the experiment using quantum particles. Previously, it didn't matter what our measuring device was, and how it worked. What solely mattered, was the fact that Alice and Bob were to (somehow) measure different properties of their particles. But now that we want to see what quantum mechanics predicts, we need to take into consideration the exact experimental apparatus and particles used. So, instead of generally talking about

"objects" and "measuring properties", we will analyse a concrete example of which the exact details are known and describable by quantum theory.

We will use the experimental setup depicted Figure 2.1, where the objects emitted will be spin-$\frac{1}{2}$ particles and the detectors will be Stern-Gerlach apparatuses that will measure some spin component of the particle. The total Hilbert space of Alice's and Bob's particles, where the quantum states of spin live in, is $H_A \otimes H_B$, where the subspaces are of dimension two, i.e. $\dim H_A = \dim H_B = 2$, spanned by $\{|\uparrow\rangle, |\downarrow\rangle\}$.

The mean value of measurement outcomes is described, in quantum theory, by the well-known observables. Specifically, if we want to measure the spin in some direction $\hat{n}$, we define the hermitian operator whose eigenstates are definite spin states pointing that direction. For example, if that direction $\hat{n}$ is defined to be simply the z-axis, then our observable will be the Pauli matrix

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.35}$$

defined in the representation $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. If the quantum system is described by the quantum state $|\psi\rangle$, the mean value of the measurement outcomes of this spin component of the particle will be

$$\langle\psi| \sigma_z |\psi\rangle . \tag{2.36}$$

But, if we are to use Bell's inequality, we will also need mean values of measurement outcomes of spin components rotated with respect to the predefined z-axis, which correspond to the "rotated" observable,

$$\hat{n} \cdot \vec{\sigma} = \begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}, \tag{2.37}$$

where $\hat{\sigma}_i$ are Pauli's matrices, and

$$\hat{n} = \begin{pmatrix} \sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta \end{pmatrix} \tag{2.38}$$

is the direction of the spin component being measured (which is proportional to the direction of Stern-Gerlach apparatus's magnetic field). The corresponding mean value of the measurements would be

$$\langle\psi| \hat{n} \cdot \vec{\sigma} |\psi\rangle . \tag{2.39}$$

In the following, we will consider the xy-plane with $\phi = 0$. Alice will measure the observable

$$\hat{A}(\theta_A) = (\hat{\sigma}_z \cos\theta_A + \hat{\sigma}_x \sin\theta_A) \otimes I_B, \tag{2.40}$$

acting only on the Hilbert space H_A of her particle, and Bob will measure

$$\hat{B}(\theta_B) = I_A \otimes (\hat{\sigma}_z \cos\theta_B + \hat{\sigma}_x \sin\theta_B) . \tag{2.41}$$

Suppose that the two particles emitted by the Source, are prepared in the singlet state

$$|\psi\rangle_{AB} = \frac{1}{\sqrt{2}} (|\uparrow\rangle_A \otimes |\downarrow\rangle_B - |\downarrow\rangle_A \otimes |\uparrow\rangle_B) , \tag{2.42}$$

which is an entangled state. If we run the experiment N times, and each time the particles are prepared in this state, while Alice and Bob measure the observable $\hat{A}(\theta_A) \otimes \hat{B}(\theta_B)$, the mean value of their joint measurements will approach the quantum mechanical value

$$_{AB}\langle\psi|\,\hat{A}(\theta_A) \otimes \hat{B}(\theta_B)\,|\psi\rangle_{AB}. \tag{2.43}$$

Note that this observable can be measured, if Alice rotate her Stern-Gerlach apparatus so that its magnetic field will point to the direction corresponding to $\phi = 0$ and $\theta = \theta_A$, while Bob will rotate his apparatus to the direction $\phi = 0$ and $\theta = \theta_B$. The alignment of the axes, with respect to which the angles ϕ and θ are defined, has been pre-agreed between Alice and Bob, so that it will be the same in both sides. Let us comment on another point as well. Remember our discussion in the previous section. We emphasized the fact that, out of the total N times we run the experiment (i.e. N pairs of particles are emitted), we measure the observable (2.43) less times, e.g. $M < N$. So, the experimental formula of the quantum mechanical value

$$_{AB}\langle\psi|\,\hat{A}(\theta_A) \otimes \hat{B}(\theta_B)\,|\psi\rangle_{AB} \approx \frac{1}{M}\sum_{i=1}^{M} A_i(\theta_A)\, B_i(\theta_B). \tag{2.44}$$

Now let's return to the evaluation of the quantum mechanical prediction for Bell's inequality. Comparing equations (2.43), (2.44) with (2.33), we infer that

$$\langle S\rangle \approx {}_{AB}\langle\psi|\,\hat{S}|\psi\rangle_{AB}, \tag{2.45}$$

where the quantity $\langle S\rangle$ is Eq. (2.33), and we also defined the *CHSH* observable,

$$\hat{S} = \hat{A}(a_1) \otimes \hat{B}(b_1) + \hat{A}(a_1) \otimes \hat{B}(b_2) + \hat{A}(a_2) \otimes \hat{B}(b_1) - \hat{A}(a_2) \otimes \hat{B}(b_2). \tag{2.46}$$

For simplicity, let us make the following choice of angles,

$$\begin{aligned} a_1 &= 0, \quad a_2 = 2\theta \\ b_1 &= \theta, \quad b_2 = -\theta. \end{aligned} \tag{2.47}$$

Substituting the expressions of $\hat{A}(\theta_A)$ and $\hat{B}(\theta_B)$ in $\hat{S}$, as well as the matrix representation of the Pauli matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.48}$$

we find

$$S_\theta = \begin{pmatrix} 2\cos\theta & 2\cos 2\theta \sin\theta & 0 & 4\cos\theta\sin^2\theta \\ 2\cos 2\theta \sin\theta & -2\cos\theta & 4\cos\theta\sin^2\theta & 0 \\ 0 & 4\cos\theta\sin^2\theta & -2\cos\theta & -2\cos 2\theta \sin\theta \\ 4\cos 2\theta\sin^2\theta & 0 & -2\cos 2\theta \sin\theta & 2\cos\theta \end{pmatrix}. \tag{2.49}$$

Finally, the mean value of this observable, in the singlet state (2.45), is

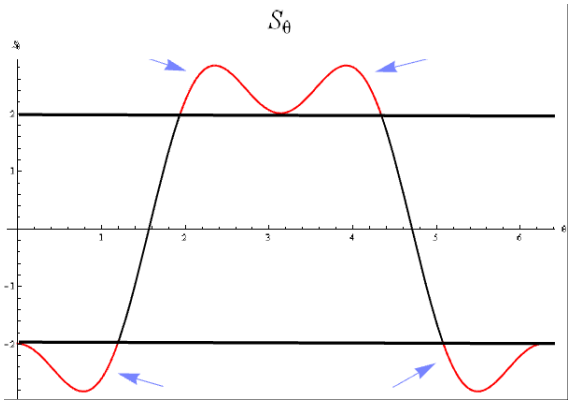

Figure 2.3: We have plotted the CHSH mean value $\langle S_\theta \rangle$ as predicted from quantum theory, Eq. (2.50), for various angles θ. We clearly see a violation of Bell's inequality, denoted in red, since the mean value exceeds the limits $-2 \leq \langle S_\theta \rangle \leq 2$, imposed by local realism. Thus, quantum theory violates local realism and, also, completely agrees with the experiment.

$$\langle S_\theta \rangle_{QM} = \frac{1}{2}\left(-4\cos\theta - 8\cos\theta \sin^2\theta\right). \tag{2.50}$$

It's easy to see that the maximum value of this quantity is

$$\left|\langle S_\theta \rangle_{QM}\right|_{\max} = 2\sqrt{2} > 2, \tag{2.51}$$

in contrast to Bell's inequality (2.26). In Figure 2.3 we have plotted this mean value $\langle S_\theta \rangle_{QM}$, as predicted by quantum theory, with respect to various angles θ. The violation of local realism is clearly visible for some angles.

2.3.6 Cirel'son's inequality

Previously, we saw that quantum theory violates the CHSH inequality if the particles are prepared in a singlet state, and that this violation comes to its maximum value $2\sqrt{2}$ for some angles. But this violation comes from the particular singlet state, however there are infinite, in number, quantum states in the Hilbert space. Could any of these states produce an even larger violation? Cirel'son [21] investigated this problem, and we give a small proof here showing that the violation $2\sqrt{2}$ is, actually, the largest violation allowed by quantum theory.

Consider the CHSH observable (2.46), which we repeat here for convenience,

$$\hat{S} = \hat{A}(a_1)\hat{B}(b_1) + \hat{A}(a_1)\hat{B}(b_2) + \hat{A}(a_2)\hat{B}(b_1) - \hat{A}(a_2)\hat{B}(b_2). \tag{2.52}$$

This operator squared can be brought to the following form,

$$\hat{S}^2 = 4 + \left[\hat{A}(a_1), \hat{A}(a_2)\right] \otimes \left[\hat{B}(b_1), \hat{B}(b_2)\right], \tag{2.53}$$

where we assumed the properties

$$\begin{aligned} \hat{A}(a_1)^2 &= \hat{A}(a_2)^2 = \hat{1}_A, \\ \hat{B}(b_1)^2 &= \hat{B}(b_2)^2 = \hat{1}_B, \end{aligned} \tag{2.54}$$

and introduced the commutator $[a,b]=ab-ba$. The norm of the operator $\hat{S}^2$, defined as $\left\|\hat{S}^2\right\|=\sup\left(\frac{\sqrt{\langle u|\hat{S}^2|u\rangle}}{\sqrt{\langle u|u\rangle}}\right)$, is found to be bounded by

$$\begin{aligned}\left\|\hat{S}^2\right\| &= \left\|4+\left[\hat{A}\left(a_1\right),\hat{A}\left(a_2\right)\right]\otimes\left[\hat{B}\left(b_1\right),\hat{B}\left(b_2\right)\right]\right\| \\ &\leq 4+\left\|\left[\hat{A}\left(a_1\right),\hat{A}\left(a_2\right)\right]\otimes\left[\hat{B}\left(b_1\right),\hat{B}\left(b_2\right)\right]\right\| \\ &\leq 4+\left\|\left[\hat{A}\left(a_1\right),\hat{A}\left(a_2\right)\right]\right\|\cdot\left\|\left[\hat{B}\left(b_1\right),\hat{B}\left(b_2\right)\right]\right\| \\ &\leq 8,\end{aligned} \tag{2.55}$$

where we used various identities of the norm that can be found, for example, in [8], and also made use of

$$\left\|\left[\hat{A}\left(a_1\right),\hat{A}\left(a_2\right)\right]\right\|\leq 2,\quad \left\|\left[\hat{B}\left(b_1\right),\hat{B}\left(b_2\right)\right]\right\|\leq 2. \tag{2.56}$$

Since, $\left\|\hat{S}\right\|^2\leq\left\|\hat{S}^2\right\|$, it holds that

$$\left\|\hat{S}\right\|\leq 2\sqrt{2}. \tag{2.57}$$

This result is important for, at least, two reasons. First of all, it says that, the mean value of $\hat{S}$ cannot exceed the maximum bound $2\sqrt{2}$ no matter what quantum state the pair of particles are described of. This is guaranteed thanks to the fact, that, the norm of $\hat{S}$ is defined as the maximum mean value of $\hat{S}$ over all possible quantum states in the Hilbert space, and the result (2.57) has been proven for the norm $\left\|\hat{S}\right\|$. The second reason is Eq. (2.55), which can be brought in the form

$$\left\|\hat{S}\right\|\leq\sqrt{4+\left\|\left[\hat{A}\left(a_1\right),\hat{A}\left(a_2\right)\right]\right\|\cdot\left\|\left[\hat{B}\left(b_1\right),\hat{B}\left(b_2\right)\right]\right\|}. \tag{2.58}$$

Notice that if one of the commutators involved is zero, i.e. one of the parties chooses to measure between commuting observables, then we get the *classical* result $\left\|\hat{S}\right\|\leq 2$. This is natural because, in that case, the quantum states in the superposition would not be able to interfere with each other. Remember that the commutator determines the lower bound in the uncertainty of our measurements,

$$\langle\Delta A\left(a_1\right)\rangle\cdot\langle\Delta A\left(a_2\right)\rangle\geq\frac{1}{2}\left|\left\langle\left[\hat{A}\left(a_1\right),\hat{A}\left(a_2\right)\right]\right\rangle\right|. \tag{2.59}$$

2.4 Why is Bell's inequality violated?

This is a long-standing question that no one can answer with certainty. What is the false assumption; reality? locality? ..or both? Here we will only give a few insights on why quantum mechanics violate Bell's inequality.

2.4.1 Implications of non-locality

First of all, let us see how is the CHSH inequality going to change if we allow non-local correlations; i.e. if we allow Alice's measurement result to depend on Bob's and vice versa. For a single photon pair j, the *local* CHSH inequality, (2.29),reads

$$\begin{aligned} S_j|_{local} &= A_j(a_1)B_j(b_1) + A_j(a_1)B_j(b_2) + A_j(a_2)B_j(b_1) - A_j(a_2)B_j(b_2) \\ &= \pm 2. \end{aligned} \tag{2.60}$$

If we allow interdependence between Alice's and Bob's measurement results, the following changes will occur,

$$A_j(a_1)B_j(b_1) \rightarrow A_j(a_1,b_1)B_j(a_1,b_1) \tag{2.61}$$
$$A_j(a_1)B_j(b_2) \rightarrow A_j(a_1,b_2)B_j(a_1,b_2) \tag{2.62}$$
$$A_j(a_2)B_j(b_1) \rightarrow A_j(a_2,b_1)B_j(a_2,b_1) \tag{2.63}$$
$$A_j(a_2)B_j(b_2) \rightarrow A_j(a_2,b_2)B_j(a_2,b_2). \tag{2.64}$$

So, in general, $A_j(a_1,b_1)$ will be different from $A_j(a_1,b_2)$, since there is a dependence on what Bob measured. The new, non-local, version of S_j will be

$$\begin{aligned} S_j|_{non-local} = A_j(a_1,b_1)B_j(a_1,b_1) + A_j(a_2,b_1)B_j(a_2,b_1) + \\ + A_j(a_1,b_2)B_j(a_1,b_2) - A_j(a_2,b_2)B_j(a_2,b_2). \end{aligned} \tag{2.65}$$

It's easy to see, now, that the maximum value of this quantity is

$$S_j|^{MAX}_{non-local} = \pm 4, \tag{2.66}$$

leading to

$$-4 \leq \left\langle S_j|_{non-local} \right\rangle \leq 4. \tag{2.67}$$

The quantum mechanical value is within this range, and this is why the quantum mechanical correlations, that violate the CHSH inequality, are known as non-local correlations. But, doesn't this non-locality, that we allowed in (2.65), violate relativistic causality? This problem was investigated by Popescu and Rohrlich [22], while searching for a way to derive quantum theory from two axioms: i) Relativistic causality ii) Non-locality. They found that there exist possible theories which are non-local, satisfying (2.67), yet satisfy relativistic causality, since these non-local correlations can be "read" only after the two parties communicate their results to each other. In the following, we will examine two effects of quantum theory that cause the violation of Bell's inequality. A very nice discussion on this issue can be found in [23], [24].

2.4.2 Quantum interference

In Section 2.3.5, we used an entangled state, the singlet state, to violate the CHSH inequality. But what quantum states are capable of violation? It has been proven in [25], that all non-product states, also known as *entangled* states, violate Bell's inequality. So, *any* entangled pure state of two qubits give non-local correlations. Let us see why.

Consider, at first, a *separable* mixed state which is a 50%-50% mixture of the bipartite quantum states $|\uparrow\downarrow\rangle \equiv |\psi_1\rangle\,, \quad |\downarrow\uparrow\rangle \equiv |\psi_2\rangle$, namely

$$\begin{aligned}\hat{\rho} &= \frac{1}{2}\,|\psi_1\rangle\,\langle\psi_1| + \frac{1}{2}\,|\psi_2\rangle\,\langle\psi_2| \\ &= \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.\end{aligned} \tag{2.68}$$

This state can be created via *LOCC*, and its correlations can be described by a local hidden variables model[26]. We will see that such a statistical mixture cannot violate the CHSH inequality, and this is useful in order to realize what makes entangled quantum states so special. Let us calculate the mean value of $\hat{S}_\theta$ with respect to this density matrix,

$$\begin{aligned}\left\langle \hat{S}_\theta \right\rangle_{\hat{\rho}} &= Tr\left(\hat{\rho}\hat{S}_\theta\right) \\ &= \frac{1}{2}\,\langle\psi_1|\,\hat{S}_\theta\,|\psi_1\rangle + \frac{1}{2}\,\langle\psi_2|\,\hat{S}_\theta\,|\psi_2\rangle \\ &= -2\cos\theta.\end{aligned} \tag{2.69}$$

Consequently, the CHSH inequality is respected. Notice that in this mixture, the two states $|\psi_1\rangle$ and $|\psi_2\rangle$ cannot interfere with each other, the density matrix has no non-diagonal terms.

Let us, now, consider a superposition of these two states, having the weight as in the above mixture,

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\psi_1\rangle + |\psi_2\rangle\right). \tag{2.70}$$

The difference, now, is that the states $|\psi_i\rangle$ can interfere with each other leading to genuine quantum effects. In particular, the mean value of $\hat{S}_\theta$, with respect to $|\psi\rangle$, is

$$\begin{aligned}\left\langle \hat{S}_\theta \right\rangle_{\psi} &= \frac{1}{2}\,\langle\psi_1|\,\hat{S}_\theta\,|\psi_1\rangle + \frac{1}{2}\,\langle\psi_2|\,\hat{S}_\theta\,|\psi_2\rangle + \frac{1}{2}\,\langle\psi_1|\,\hat{S}_\theta\,|\psi_2\rangle + \frac{1}{2}\,\langle\psi_2|\,\hat{S}_\theta\,|\psi_1\rangle \\ &= \left\langle \hat{S}_\theta \right\rangle_{\hat{\rho}} + \underbrace{\frac{1}{2}\,\langle\psi_1|\,\hat{S}_\theta\,|\psi_2\rangle + \frac{1}{2}\,\langle\psi_2|\,\hat{S}_\theta\,|\psi_1\rangle}_{\text{interference}} \\ &= -2\cos\theta - \underbrace{2\sin 2\theta \sin\theta}.\end{aligned} \tag{2.71}$$

We can clearly see that it's the interference terms that make the magnitude of this mean value large than 2. Responsible for the interference is the entanglement between the two particles, however just the entanglement is not enough to cause the violation. In order for the interference terms to give non-zero contribution, the observable $\hat{S}_\theta$ must include non-commutative observables so that the orthogonal states $|\psi_i\rangle$ will not cancel each other out. So, we come to the second important cause of the violation, the non-commutativity of the involved observables.

2.4.3 Non-commutativity of observables

A necessary but no sufficient condition for the CHSH inequality to be violated, is to involve non-commutative observables. We encountered this fact in our discussion of Cirel'son's inequality (2.58). In order to understand this better, let us consider the following example.

The eigenvalues of the Pauli matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

are simply ± 1. If we measured each of these two observables separately, ± 1 would be the only possible results. Now we add them, and form another observable

$$S \equiv \sigma_x + \sigma_z. \tag{2.72}$$

Question: The possible values of S are $\{-2, 0, 2\}$?
Answer: No. The eigenvalues of S are not, in general, the sum of the eigenvalues of the non-commutative observables σ_x, σ_z. In particular, if we calculate S's eigenvalues we will find $\pm\sqrt{2}$! This phenomenon is due to the fact, that, non-commutative observables do not have certain values simultaneously. For example, when σ_x has a definite value then σ_z will correspond to a quantum superposition of it's possible values, whatever this 'superposition' means in quantum theory. So, in some sense, citing the words of Tanimura [24], *in quantum mechanics* $1 + 1$ *is not 2 but* $\sqrt{2}$.

Now, let us make the connection between the CHSH formulation and this illustrative example. The quantity (2.52), namely,

$$\hat{S} = \hat{A}(a_1)\hat{B}(b_1) + \hat{A}(a_1)\hat{B}(b_2) + \hat{A}(a_2)\hat{B}(b_1) - \hat{A}(a_2)\hat{B}(b_2),$$

involves four non-commutative observables. Each of the observables, when measured in their eigenstates, acquire a definite value ± 1. However, when we actually measure one of the observables, then the rest of them will have not a definite value. Quantum mechanics tells us, that, they will be in a quantum superposition of their values, as we saw in the previous example. This quantum superposition has one crucial consequence: The arithmetic rule of simply adding the possible eigenvalues values of non-commutative observables, doesn't hold for quantum objects, $1 + 1$ equals $\sqrt{2}$ (symbolically), not 2. However, non-commutativity, by itself, is not enough in order to violate Bell's inequality, it also needs entangled states. The use of separable, i.e. product, states will not work. And, vice versa, entanglement by itself is not capable for a violation, it needs to be combined with the non-commutativity of the observables measured.

So, what may we possibly conclude from all this? The most safe conclusion that we can draw is, that, no *local hidden variable model (LHVM)* can account for all quantum correlations of composite quantum systems. In our derivation of the CHSH inequality, we didn't write down any hidden variables explicitly but we we used this concept implicitly, when we assumed that unperformed experiments have results (assumption of reality). But, are these quantum correlations, that violate Bell's inequality, non-local? In the literature we usually find this nomenclature, but this is kind of misleading. The word 'non-locality' is only used to express the fact no *Local HVM* can account for these correlations. But which exactly is the false assumption, locality or reality (or both), is not clear.

2.5 Uses of quantum entanglement

Now, that we have understood what entanglement is, let us see what entanglement can actually do. Besides any philosophical interest about it, wondering whether nature is local and realistic, entanglement has some important practical applications in Quantum Information and Quantum Cryptography. It is used as an invaluable resource for doing things that are not classically possible. In the following, we will briefly examine some of them.

2.5.1 Quantum Teleportation

One of the most spectacular applications of quantum entanglement, is the ability that it gives us to teleport unknown quantum states from one place to the other, ..instantly! In order to better appreciate this, let us first think what are our other options. Assume that Alice has, in her possession, a qubit in an *unknown* pure state $|\psi\rangle$, and she wants to give this state $|\psi\rangle$ to Bob. What are her options?

Option (A): Transport it to Bob. Why not do the *obvious*? Alice takes her car and her qubit, and goes over to Bob's place to, simply, give it to him! There are at least to problems with this approach. First and foremost, it's the problem of decoherence. An actual transport of a quantum state will unavoidably increase the possibility that the qubit will interact with the environment. As a result, the state $|\psi\rangle$ will be altered, any quantum superpositions will be lost, and Bob will finally receive the wrong state. But, suppose that Alice can completely isolate her qubit, so that it does not interact with the environment during the journey. Now the problem would be to actually travel over to Bob's place! Perhaps Alice and Bob live far away from each other, they could live from different continents to different planets in the solar system! Then an actual travel, for just a qubit, is highly impractical. What other options does Alice have?

Option (B): Measure it. Alice also has the option to actually measure and find what $|\psi\rangle$ is, and communicate the result to Bob. Then, Bob will be able to reproduce this state in his lab. There are two problems with this approach: If you want to find a quantum state, e.g. the a and b of $|\psi\rangle = a\,|0\rangle + b\,|1\rangle$, you need to do measure many systems prepared in this exact state. So, if you have only one qubit in this state, instead of many, finding out what this quantum state is, is simply impossible. But if you had many qubits N in this state, then you would able to measure it via the process of *quantum state tomography* and communicate the results to Bob (which are *many bits* of information!). However, many experimental and statistical errors will enter your final calculations! Let alone the fact that Bob would need to, somehow, prepare that state in his lab.

Option (C): *Teleport it!* Options A and B are impractical, for various reasons. Option C is a more exotic and efficient way to send quantum information (i.e. send states of quantum bits, instead of classical bits) to another party. Suppose that Alice and Bob

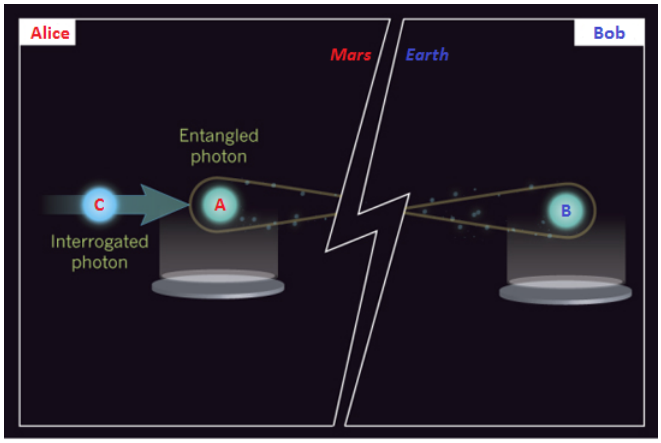

Figure 2.4: The necessary setup for quantum teleportation is depicted. Alice and Bob, separated by an arbitrarily large distance, share an entangled pair of qubits AB (e.g. photons). Alice wants to teleport the unknown quantum state, of her second qubit C, to Bob's qubit B, by taking advantage of the existing entanglement.

share an entangled pair of qubits AB in the quantum state,

$$\left|\phi^{+}\right\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|00\rangle_{AB} + |11\rangle_{AB}\right), \tag{2.73}$$

which they had created in the past (perhaps a couple of years ago). Alice wants Bob to acquire the unknown quantum state

$$|\psi\rangle_{C} = a\,|0\rangle + b\,|1\rangle\,, \tag{2.74}$$

where the amplitudes a, b are unknown, 'carried' by the qubit C that she possesses together with qubit A in her lab. She remembers that Bob and herself share the entangled pair AB, so Alice is going to use this entanglement as a *resource*, in order to teleport the state $|\psi\rangle$, of her qubit C, to Bob! The situation is beautifully depicted in Figure 2.4. Now, let us see how is going to accomplish this.

The joint quantum state of the three qubits is a product state,

$$\begin{aligned} |\psi\rangle_{C} \otimes \left|\varphi^{+}\right\rangle_{AB} &= (a|0\rangle_{C} + b|1\rangle_{C}) \otimes \frac{1}{\sqrt{2}}\left(|00\rangle_{AB} + |11\rangle_{AB}\right) \\ &= \frac{1}{\sqrt{2}}\left(a|000\rangle_{CAB} + a|011\rangle_{CAB} + b|100\rangle_{CAB} + b|111\rangle_{CAB}\right), \end{aligned} \tag{2.75}$$

In the next state, Alice will have to make a joint measurement of her qubits C and A, in the so-called Bell basis, i.e. the following four mutually orthogonal states

$$\left|\psi^{\pm}\right\rangle_{CA} = \frac{1}{\sqrt{2}}\left(|01\rangle_{CA} \pm |10\rangle_{CA}\right) \tag{2.76}$$

$$\left|\varphi^{\pm}\right\rangle_{CA} = \frac{1}{\sqrt{2}}\left(|00\rangle_{CA} \pm |11\rangle_{CA}\right). \tag{2.77}$$

In order to make the result more obvious, we will re-write the join quantum state of qubits ABC a little bit differently, but in an equivalent way, so that the dependence on

the Bell basis will be obvious. Equivalently, from (2.75), we have

$$\begin{aligned}
|\psi\rangle_C \otimes |\varphi^+\rangle_{AB} &= \frac{1}{2}a\left(|\varphi^+\rangle_{CA} + |\varphi^-\rangle_{CA}\right)|0\rangle_B + \frac{1}{2}a\left(|\psi^+\rangle_{CA} + |\psi^-\rangle_{CA}\right)|1\rangle_B \\
&+ \frac{1}{2}b\left(|\psi^+\rangle_{CA} - |\psi^-\rangle_{CA}\right)|0\rangle_B + \frac{1}{2}b\left(|\varphi^+\rangle_{CA} - |\varphi^-\rangle_{CA}\right)|1\rangle_B \\
&= \frac{1}{2}|\varphi^+\rangle_{CA}\left(a|0\rangle_{\mathrm{B}} + b|1\rangle_{\mathrm{B}}\right) + \frac{1}{2}|\psi^+\rangle_{CA}\left(a|1\rangle_{\mathrm{B}} + b|0\rangle_{\mathrm{B}}\right) \\
&+ \frac{1}{2}|\psi^-\rangle_{CA}\left(a|1\rangle_{\mathrm{B}} - b|0\rangle_{\mathrm{B}}\right) + \frac{1}{2}|\varphi^-\rangle_{CA}\left(a|0\rangle_{\mathrm{B}} - b|1\rangle_{\mathrm{B}}\right) \\
&= \frac{1}{2}|\varphi^+\rangle_{CA} \otimes |\psi\rangle_{\mathrm{B}} + \frac{1}{2}|\psi^+\rangle_{CA} \otimes \left(\hat{\sigma}_x|\psi\rangle_{\mathrm{B}}\right) \\
&+ \frac{1}{2}|\psi^-\rangle_{CA} \otimes \left(-i\hat{\sigma}_y|\psi\rangle_{\mathrm{B}}\right) + \frac{1}{2}|\varphi^-\rangle_{CA} \otimes \left(\hat{\sigma}_z|\psi\rangle_{\mathrm{B}}\right).
\end{aligned} \tag{2.78}$$

When Alice performs the measurement on the basis $\{|\varphi^{\pm}\rangle_{CA}, |\psi^{\pm}\rangle_{CA}\}$, she will acquire one of the four possible outcomes. As you can see from (2.77), if Alice's result is $|\varphi^+\rangle_{CA}$, then Bob's qubit will be in the exact state $|\psi\rangle_{\mathrm{B}} = a|0\rangle_{\mathrm{B}} + b|1\rangle_{\mathrm{B}}$ Alice wanted to teleport! For the rest of the results, $|\varphi^-\rangle_{CA}$, $|\psi^{\pm}\rangle_{CA}$ Bob's state is *almost* what Alice wanted to teleport. In order to acquire the exact state, Bob needs perform one of the following operations on his qubit, depending on Alice's result:

$$|\varphi^+\rangle_{CA} \rightarrow \underbrace{\hat{1}_B}\cdot|\psi\rangle_{\mathrm{B}} = |\psi\rangle_{\mathrm{B}} \tag{2.79}$$

$$|\psi^+\rangle_{CA} \rightarrow \underbrace{\hat{\sigma}_x}\cdot\left(\hat{\sigma}_x|\psi\rangle_{\mathrm{B}}\right) = |\psi\rangle_{\mathrm{B}} \tag{2.80}$$

$$|\psi^-\rangle_{CA} \rightarrow \underbrace{\hat{\sigma}_y}\cdot\left(\hat{\sigma}_y|\psi\rangle_{\mathrm{B}}\right) = |\psi\rangle_{\mathrm{B}} \tag{2.81}$$

$$|\varphi^-\rangle_{CA} \rightarrow \underbrace{\hat{\sigma}_z}\cdot\left(\hat{\sigma}_z|\psi\rangle_{\mathrm{B}}\right) = |\psi\rangle_{\mathrm{B}}. \tag{2.82}$$

Alice needs only to communicate her measurement result to Bob, i.e. whether she got $|\varphi^+\rangle_{CA}, |\psi^+\rangle_{CA}, |\psi^-\rangle_{CA}$ or $|\varphi^-\rangle_{CA}$. Notice that these states, (2.76)-(2.77), have no information about the amplitudes a,b of the unknown state (2.74)! Whatever this unknown state is (infinite possibilities), Alice will always communicate one of these four results, so it's wrong to thing that she actually sends any information about $|\psi\rangle$. Yet, this little information (2 classical bits to be exact) that she sends to Bob, is enough to help him acquire the original unknown state! This procedure is known as *teleportation of quantum information*. What's extraordinary about it, is that those non-local correlations that violated Bell's inequality in the previous Section, appearing like an *action at a distance*, can actually teleport quantum information from one place to the other instantly! The fact that Bob needs two bits of information from Alice, in order to "unlock" the unknown state, is what saves causality. Finally, when we investigated Bell's inequalities previously, we were not sure in the end whether it's locality or reality (i.e. counter-factuality) that fails in nature. Quantum teleportation seems to suggest that locality does not hold in nature.

Another point that we would like to point out is the following. In order to achieve the perfect teleportation we used the singlet (2.73), one of the Bell states. These states

are known as maximally entangled states for reasons we will discuss later on in Section 2.8. But what if we used another quantum state of the more general form

$$|\varphi\rangle_{AB} = \cos\theta|00\rangle_{AB} + \sin\theta|11\rangle_{AB}, \tag{2.83}$$

would teleportation still be possible? Quite recently it was shown [27], that, using *two* auxiliary qubits you can achieve a probabilistic teleportation, i.e. there is a probability that teleportation will either work or fail but we are certain when it does. Ofcourse, in the limit $\theta \to \frac{\pi}{4}$ the chance of success tends to unity. What about the teleportation capabilities of entangled mixed states? An example of such states, are the so-called Werner states [26] with a density matrix of the form

$$\hat{\rho}_{AB} = \frac{1}{8}\hat{1}_{AB} + \frac{1}{2}\left|\psi^-\right\rangle_{AB}{}_{AB}\left\langle\psi^-\right|. \tag{2.84}$$

Popescu showed [28] that teleportation using such a state is possible but not perfect, i.e. the final teleported state to Bob does not exactly match the state Alice wanted to sent, but is close to it. The concept describing how close one state is to the other is called *fidelity*, and is defined as

$$F = |\langle \textit{input state} \mid \textit{teleported state}\rangle|^2. \tag{2.85}$$

For example, a perfect teleportation results to $F = 1$ since the teleported state equals the initial one, while a teleportation using (2.84) leads to $F < 1$. We think that no entangled mixed state can achieve $F = 1$, but we are not aware of such a general proof.

Some Remarks:

In Section 1.3.4, where we talked about ensembles and density matrices, we mentioned that a single mixed density matrix can describe infinitely many ensembles. Let us see this feature in action, right here in the teleportation procedure.

Initially, Alice and Bob entangled pair is in the quantum state

$$\left|\varphi^+\right\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|00\rangle_{AB} + |11\rangle_{AB}\right). \tag{2.86}$$

If we calculate the reduced quantum state of Bob's qubit, by summing over Alice's degrees of freedom, we will find

$$\hat{\rho}_{\mathrm{B}} = \frac{1}{2}|0\rangle_{\mathrm{BB}}\langle 0| + \frac{1}{2}|1\rangle_{\mathrm{BB}}\langle 1| = \frac{1}{2}\hat{1}_{\mathrm{B}}. \tag{2.87}$$

Now, when Alice brings in her other qubit C and jointly measures both qubits CA the whole quantum state collapses, including Bob's qubit. In particular, Bob's qubit collapses in a pure state, $|\psi\rangle_{\mathrm{B}}D$ or $\hat{\sigma}_i|\psi\rangle_{\mathrm{B}}$, which is *almost* the same with the unknown state! However, in order for causality not be violated, Bob's reduced state should still be a maximally mixed state (2.87), even after Alice's measurement! But is it? Let's find out.

Just before Alice's measurement, the joint quantum state is,

$$\begin{aligned}|\psi\rangle_C \otimes \left|\varphi^+\right\rangle_{AB} = \frac{1}{2}\left|\varphi^+\right\rangle_{CA} \otimes |\psi\rangle_{\mathrm{B}} + \frac{1}{2}\left|\psi^+\right\rangle_{CA} \otimes (\hat{\sigma}_x|\psi\rangle_{\mathrm{B}}) \\ + \frac{1}{2}\left|\psi^-\right\rangle_{CA} \otimes (-i\hat{\sigma}_y|\psi\rangle_{\mathrm{B}}) + \frac{1}{2}\left|\varphi^-\right\rangle_{CA} \otimes (\hat{\sigma}_z|\psi\rangle_{\mathrm{B}}).\end{aligned} \tag{2.88}$$

If we calculate Bob's reduced state, by summing over the degrees of freedom of C and A, we will find

$$\begin{aligned}\hat{\rho}_{\mathrm{B}} &= \frac{1}{4}|\psi\rangle_{\mathrm{BB}}\langle\psi| + \frac{1}{4}\hat{\sigma}_x|\psi\rangle_{\mathrm{BB}}\langle\psi|\hat{\sigma}_x + \\ &+ \frac{1}{4}\hat{\sigma}_y|\psi\rangle_{\mathrm{BB}}\langle\psi|\hat{\sigma}_y + + \frac{1}{4}\hat{\sigma}_z|\psi\rangle_{\mathrm{BB}}\langle\psi|\hat{\sigma}_z \\ &= \frac{1}{2}\hat{1}_{\mathrm{B}}.\end{aligned} \tag{2.89}$$

Notice that the two ensembles (2.87) and (2.89) are completely equivalent! There are infinitely many states $|\psi\rangle_{\mathrm{B}} = a|0\rangle_{\mathrm{B}} + b|1\rangle_{\mathrm{B}}$, so Bob's reduced density matrix is capable of describing infinitely many ensembles, no matter what quantum state Alice wants to teleport. As we said previously, without the *key* 2-bit information from Alice, Bob cannot distinguish any particular state from his mixture. Viewed from this scope, Alice's information allows Bob to extract a specific pure state out of his maximally mixed state.

Finally, let us note that even a mixed state can be teleported, and in Part II of this project we will see that continuous variable states can be teleported as well.

2.5.2 Other

We analysed, in quite a detail, the procedure of quantum teleportation since it's a great illustration of the capabilities of the non-local correlations of entanglement, and it's also of great importance in the field of quantum information. In this section, we will briefly report on other uses of entanglement giving relevant references to the reader, for further research.

Double density coding Imagine two parties, Alice and Bob, that want to communicate by exchanging encoded information, i.e. bits or qubits. If Alice sent a single bit to Bob, then Bob will acquire 1 bit of information. But what about qubits, that can be in superposition of states? Well, it can by seen, that, a single qubit by itself cannot carry more that 1 bit of information, due to the fact that Bob's measurement destroys the state. However, Bennett *et. al.* [29] found that by using, already established, entanglement between Alice and Bob as a resource, a single qubit sent down the channel can carry 2 bits of information! So, entanglement can be used as a resource in order to densely encode information, twice as much as is classically possible.

Quantum key distribution Entanglement opened up a new field, namely that of Quantum Cryptography. In cryptography, a major problem for two distant parties is to establish a secret cryptographic key, in order to communicate secretly. The non-local correlations of entanglement supply them with the possibility of secure key distribution, with the laws of quantum mechanics making *almost* impossible for someone to eavesdrop. For more information and references, check the following complete review of quantum cryptography [30].

Other

• Entanglement is, also, an invaluable resource in the field of Quantum Computation. Shor's famous factorization quantum algorithm [31] relies on entanglement.

• Moreover, new quantum technologies, like ghost imaging [32], rely on this peculiar quantum property. This technique allows us to image objects with a resolution, or other imaging criteria, that is beyond what is classically possible in classical optics.

• Entanglement has also been a very useful tool in the study of many-body systems. In particular, it has been shown that entanglement can be used as an indicator of a quantum phase transition in bosonic or fermionic systems [33]-[35].

• It has, also, been found to play a crucial role in explaining the bulk properties of solids [36] (e.g. magnetic susceptibility), it exists in macroscopic systems at high temperatures [37], and thus gives us a way of probing the quantum-to-classical transition.

• Last but not least, entanglement can also be used as a tool to determine spacetime parameters, such as the expansion rate of the Universe [38].

2.6 Separability Criteria

Up to now, we have seen what entanglement is and what is so special about it. Consequently, it's very important that we have a criterion to tell us whether a given quantum state is separable or entangled, so, in this section, we will introduce some important separability criteria. Before we do that, it's necessary that we understand something important.

2.6.1 Entanglement is a relative property of a quantum state

Entanglement is not an absolute property of a quantum state, it's a relative one. That is, it's relative to the specific decomposition of the Hilbert space our measurements (projections) are acting on, consequently a given quantum state may be entangled with respect to some decomposition and the same state could be separable to some other decomposition. To make things simple, let us work out a specific example.

Example Consider a pair of qubits in one of the four Bell states,

$$\left|\psi^{\pm}\right\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|01\rangle_{AB} \pm |10\rangle_{AB}\right), \quad \left|\varphi^{\pm}\right\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|00\rangle_{AB} \pm |11\rangle_{AB}\right). \tag{2.90}$$

First of all, consider the natural decomposition of the Hilbert space as $H_A \otimes H_B$ with $|i\rangle_A \in H_A$ and $|j\rangle_B \in H_B$ being the degrees of freedom of the particles A, B. That is to say, our measurements (mathematically treated as projectors $\hat{M}_i$) will project the particle's quantum state either on some state belonging to H_A or/and H_B, but not on a state being a linear superposition of both. In other words, these kind of projections that act on each particle A, B separately will project the pair's state in a product state, where the *product* is defined by the decomposition $H_A \otimes H_B$. An example of such measurements (projections) are

$$\hat{M}_{0,A} = |0\rangle_{AA}\langle 0|, \qquad \hat{M}_{1,A} = |1\rangle_{AA}\langle 1|, \tag{2.91}$$

acting on H_A, and

$$\hat{M}_{0,B} = |0\rangle_{BB}\langle 0|\,, \qquad \hat{M}_{1,B} = |1\rangle_{BB}\langle 1|\,, \tag{2.92}$$

acting on H_B. Relative to these projections/measurements, the Bell states (2.90) are entangled, since they cannot be expressed as a product state in $H_A \otimes H_B$.

However, we could have made our measurements in another basis, namely the Bell basis (2.90) that act, not on single particles, but on collective degrees of freedom. Remember that quantum theory allows to make measurements on whatever orthonormal basis we please. We re-write the Bell states in a new Hilbert space decomposition

$$|f^m\rangle \equiv |f\rangle \otimes |m\rangle\,, \quad \text{with} \quad f = \phi, \psi, \quad m = \pm, \tag{2.93}$$

that correspond to the bipartition $H_f \otimes H_m$. Let us see what such a decomposition actually means. We can either measure in the basis $\{|\varphi\rangle\,, |\psi\rangle\}$ of the first part of the bipartition, i.e. to find out whether our two particles' spins point in the same (ψ) or opposite (ϕ) direction, or we can measure in the basis $\{|\varphi\rangle\,, |\psi\rangle\}$ of the second part of the bipartition, i.e. to find out the relative sign $\pm$ of the superposition without getting any information on the alignment of the spins. These degrees of freedom are known as *collective*, since our measurements act non-locally on both particles, not on a single particle separately. Now, if our particles are in one of the Bell states (2.90), and we make measurements according to the bipartition $H_f \otimes H_m$ (instead of $H_A \otimes H_B$), then by definition (2.93) the Bell states will be product states, hence separable. On the contrary, some separable superpositions in the bipartition $H_A \otimes H_B$, such as $|x\rangle_A \otimes |y\rangle_B$ ($x, y \in \{0, 1\}$), are entangled in the new bipartition $H_f \otimes H_m$.

We saw that the same state can be considered as separable or entangled depending on the observables that we choose to measure, and conclude that entanglement is not an absolute property of a quantum state but a relative one. Hence, it's meaningless to refer to a Bell state, for example, as being entangled, without having specified the, so-called, tensor product structure that our measurements act on. Theoretically we can make measurements on whatever tensor product structure we wish, however in a real experimental setting the accessible observables are limited. So, a quantum state's (in)separability depends on what observables are actually accessible. For example, is some quantum-dot quantum computing proposals utilizing electron spins [39], it's easier experimentally to manipulate collective degrees of freedom, such as exchange interactions, than to control single spins [40].

For a complete discussion of the issues raised in the section, we refer the reader to the literature [41]-[43] and references therein. In the following sections, the tensor product structure that we will imply, will be explicitly written. For example, when we write the Bell state as

$$|\varphi^{\pm}\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|00\rangle_{AB} \pm |11\rangle_{AB}\right) = \frac{1}{\sqrt{2}}\left(|0\rangle_A \otimes |0\rangle_B \pm |1\rangle_A \otimes |1\rangle_B\right),$$

the tensor product structure implied is $H_A \otimes H_B$.

2.6.2 The PPT criterion

The first, and probably most important, separability criterion was developed by A. Peres [44]; let us see how it works. Consider a separable bipartite and, generally, mixed density

matrix

$$\hat{\rho} = \sum_i p_i \hat{\rho}_{i,A} \otimes \hat{\rho}_{i,B}. \tag{2.94}$$

Next, we consider the operation of partial transposition of $\hat{\rho}$, i.e. $\hat{\rho}^{PT}$, which is defined as the total transposition of only one of the subsystems (doesn't matter which one),

$$\hat{\rho}^{PT} = \sum_i p_i \hat{\rho}_{i,A} \otimes \hat{\rho}_{i,B}^T. \tag{2.95}$$

On a given basis, the total transposition of an operator is defined as,

$${}_B\langle n|\, \hat{\rho}_{i,B}^T |m\rangle_B = {}_B\langle m|\, \hat{\rho}_{i,B} |n\rangle_B. \tag{2.96}$$

It's straightforward to see that a totally transposed density matrix, is itself a legitimate density matrix. For a proof, we refer the reader to the Appendix A where there also is a detailed discussion on partial transposition. In this particular example, $\hat{\rho}_{i,B}^T \equiv \hat{\sigma}_{i,B}$ is a legitimate density matrix which means that

$$\hat{\rho}^{PT} = \sum_i p_i \hat{\rho}_{i,A} \otimes \hat{\sigma}_{i,B} \tag{2.97}$$

is itself a legitimate density matrix. We conclude that $\hat{\rho}^{PT}$ should only have positive eigenvalues. However, if a given density matrix $\hat{\rho}$ is entangled, and consequently cannot be written in the separable form (2.94), some of the eigenvalues of the partial transposed $\hat{\rho}^{PT}$ *could* be negative. In other words, if the partial transpose of a given density matrix has only non-negative eigenvalues then we cannot infer whether it is separable or entangled. On the other hand, if one or more eigenvalues happen to be negative, we are certain that this density matrix is entangled. This is the *Positive Partial Transposed (PPT)* criterion, and is a necessary condition for separability.

A few months later after the publication of Peres' result, the Horodecki family proved [45] that the PPT criterion is a necessary and sufficient conditions for separability, for bipartite systems with Hilbert space dimensions 2×2 and 2×3. Horodecki's contribution made PPT a very powerful and simple criterion; it can detect entanglement in arbitrary pure or mixed states of this dimension. For higher dimensions, however, the problem remains unsolved and the PPT criterion is only a necessary conditions for separability. Let us work out an example to demonstrate the use of this criterion.

Example Consider the Bell state,

$$\hat{\rho} = \left|\varphi^+\right\rangle_{AB}{}_{AB}\left\langle\varphi^+\right| = \frac{1}{2}\left(|00\rangle\langle 00| + |11\rangle\langle 11| + |00\rangle\langle 11| + |11\rangle\langle 00|\right), \tag{2.98}$$

which, in the representation $|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, $|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, admits the matrix form

$$\hat{\rho} \to \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}. \tag{2.99}$$

The total Hilbert space $H = H_A \otimes H_B$, that this state belongs to, is of dimension 2×2, so expect the PPT criterion to detect entanglement. We consider the partial transpose of $\hat{\rho}$, by taking the total transpose of the second subsystem in the basis $\{|0\rangle_B, |1\rangle_B\}$. The total transposition of B leads to the replacement

$$|00\rangle\langle 11| \to |01\rangle\langle 10|, \quad |11\rangle\langle 00| \to |10\rangle\langle 01|, \tag{2.100}$$

so the matrix form of $\hat{\rho}^{PT}$ becomes

$$\hat{\rho}^{PT} \to \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2.101}$$

The eigenvalues of this partially transposed state state are $\{-1, 1, 1, 1\}$. We observe that one of the eigenvalues, $\lambda_1 = -1$, is negative and, due to the PPT criterion, we conclude that the density matrix (2.98) is entangled.

Finally, let us mention that for Hilbert space dimensions other than 2×2 and 2×3, there are PPT entangled states, i.e. entangled states whose partial transpose has only positive eigenvalues and hence not detected by. This type of entanglement is known as *bound entanglement* and we will make a discussion about its peculiarities later on, when we'll talk about distillation of entanglement.

Other criteria

Various other separability criteria were developed after the Peres-Horodecki (PPT) criterion, for a review see [3], [4]. Let us just mention one of the most important of these criteria, namely the *CCNR* or *realignment* criterion that developed independently by Rudolph [46] and Chen *et. al.*[47]. The importance of this criterion stems from the fact, that, it detects entanglement for many states where the PPT criterion fails. However, it cannot detect all entangled state of two qubits as PPT, and therefore should be viewed as complementary to PPT.

2.6.3 Entanglement Witnesses

All the separability criteria that we examined, or mentioned, in the previous section require the knowledge of the density matrix in order to work. Imagine, however, that we are experimenting in our lab and produce a pair of particles in an unknown quantum state. We want to know whether this state is entangled, how can we do that? Here, is where the entanglement witnesses join the scene. In simple words, entanglement witness is an observable which we can measure. By measuring its mean value with respect to the unknown quantum state, we can decide whether the state is entangled if this mean value is lower than zero. Mathematically we can express the previous statement as in the following definition.

Definition 2. *We call an observable $\hat{W}$ entanglement witness if*

- $Tr\left[\hat{W}\hat{\rho}_S\right] \geq 0$ - *for all separable states $\hat{\rho}_S$,*
- $Tr\left[\hat{W}\hat{\rho}_E\right] < 0$ - *for at least one entangled state $\hat{\rho}_E$.*

In order to easier understand this concept, let us work out a specific example.

Example Consider two spin-$\frac{1}{2}$ particles coupled by a Heisenberg interaction $\hat{H} = -J\vec{\sigma}_A\vec{\sigma}_B$ where J is the coupling strength and $\vec{\sigma}$ denotes the Pauli matrices of particles A and B respectively. It's easy to see that for any separable state of the form

$$\hat{\rho}_S = \sum_i p_i \hat{\rho}_{i,A} \otimes \hat{\rho}_{i,B},$$

the absolute mean value of the Hamiltonian is

$$\begin{aligned} \left|\left\langle \hat{H} \right\rangle_{\hat{\rho}_S}\right| = \left|Tr\left[\hat{H}\hat{\rho}_S\right]\right| &= J\left|\sum_i p_i \langle\vec{\sigma}_A\rangle_{\hat{\rho}_{i,A}} \langle\vec{\sigma}_B\rangle_{\hat{\rho}_{i,B}}\right| \\ &\leq J\sum_i p_i \left|\langle\vec{\sigma}_A\rangle_{\hat{\rho}_{i,A}} \langle\vec{\sigma}_B\rangle_{\hat{\rho}_{i,B}}\right|. \end{aligned} \tag{2.102}$$

Since $\left|\langle\vec{\sigma}_A\rangle_{\hat{\rho}_{i,A}} \langle\vec{\sigma}_B\rangle_{\hat{\rho}_{i,B}}\right| \leq 1$, we find that the average value is bounded by the interaction strength,

$$\left|\left\langle \hat{H} \right\rangle_{\hat{\rho}_S}\right| \leq J, \tag{2.103}$$

for *all* separable states.

However, consider that the two particles are in the singlet state

$$\left|\psi^-\right\rangle_{AB} = \frac{1}{\sqrt{2}}\left(\left|\uparrow_z\right\rangle_A\left|\downarrow_z\right\rangle_B - \left|\downarrow_z\right\rangle_A\left|\uparrow_z\right\rangle_B\right),$$

which is an entangled state. The mean value of $\hat{H}$ with respect to this state is found to be,

$$\left\langle \hat{H} \right\rangle_{\psi^-} = {}_{AB}\left\langle\psi^-\right|\hat{H}\left|\psi^-\right\rangle_{AB} = 3J, \tag{2.104}$$

a value which is well above the bound (2.103), hence the singlet state is indeed an entangled state. This fact constitutes the Hamiltonian $\hat{H} = -J\vec{\sigma}_A\vec{\sigma}_B$ an entanglement witness, which can be measured in the lab and reveal entanglement without us knowing the quantum state of the particles.

The theory of entanglement witnesses is an indispensable tool, that was first developed by Horodecki *et. al.* [45] and Terhal [48]. Some of the important problems that have concerned the literature over the years are the construction of entanglement witnesses and their optimality. Regarding the latter, a witness W_1 is considered to be finer than W_2, if it detects all the entangled states that W_2 does. Consequently, it's natural to try and find procedures that give the *optimal* witness, i.e. the one that no other witness is finer than it. Such an investigation was carried out, for example, by Lewenstein *et. al.* in [49], [50].

2.7 Entanglement concentration/distillation

It is time that we talk about one of the most important tasks in the quantum information theory, that of entanglement concentration (or distillation), which is very relevant to our discussion of entanglement measures in the next chapter. First of all, let us state the

problem and, as a start, we will consider the quantum teleportation procedure in the real world.

In order for quantum teleportation to work, an entangled pair, distributed among the parties, should be established. But, in order to generate the entangled pair in the first place, one should have brought them together, allow them to interact, and when the entanglement is established *then* distribute the particles to Alice and Bob. The problem lies in the distribution process. Distribution means that the two entangled qubits will travel, through physical space, in order to reach Alice and Bob. However, in physical space there are other quantum systems (known as the *environment*) that might interact with the qubits, and as a result the initial pure singlet

$$\left|\psi^{-}\right\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle_A|\downarrow_z\rangle_B - |\downarrow_z\rangle_A|\uparrow_z\rangle_B\right),$$

will end up being an entangled *mixed* state $\hat{\rho}_{AB}$ (with $Tr\hat{\rho}_{AB}^2 < 1$), since the degrees of freedom of the environment are traced out. In real world experiments it's impossible to completely isolate a quantum system, so this degradation of the pure maximally entangled singlet is inevitable. When we discussed quantum teleportation, we mentioned that entangled *mixed* states are not capable of perfectly teleporting a quantum state, so it seems like we are in trouble.

The solution to this problem was given by Bennett *et. al.* in [51], [52]. In their proposal, each of the two observers, Alice and Bob, have in their possession N quantum systems coming from entangled pairs prepared in the some quantum state $\hat{\rho}$. Now, both observers carry out a specific recursive protocol, consisting of

• *local operations*: Alice and Bob are allowed to locally manipulate their particles, via either unitary transformations or generalised measurements.

• *classical communication*: The two parties are allowed to communicate with each other so that they can coordinate their (local) actions.

The protocol, consisting of a few steps, is repeated many times, and each time some of the quantum systems are being discarded due to their failure in passing the protocol. Those pairs of entangled qubits that remain, are approximately in a pure singlet state ready to be used in quantum information tasks. So, in some sense, no extra entanglement was generated but the already existing entanglement -distributed in many pairs- is concentrated (or distilled) in a fewer pairs. That is why this process is known as *entanglement concentration* or *entanglement distillation*.

Let us report some more concrete results. In [51], Bennett *et. al.* studied the simpler case where the initial independent n pairs were in a pure entangled, but not maximally entangled, state of the form

$$|\Psi\left(A,B\right)\rangle = \prod_{i=1}^{n}\left(\cos\theta\,|a_1\left(i\right)\beta_1\left(i\right)\rangle + \sin\theta\,|a_2\left(i\right)\beta_2\left(i\right)\rangle\right), \tag{2.105}$$

in other words, having n copies of

$$|\Psi_i\rangle_{AB} = \cos\theta|a_1\left(i\right)\beta_1\left(i\right)\rangle_{AB} + \sin\theta|a_2\left(i\right)\beta_2\left(i\right)\rangle_{AB}. \tag{2.106}$$

They found that the partial entanglement present in the n pairs, can be concentrated into m singlets via the aforementioned local operations and communication, asymptotically

yielding

$$\lim_{n\to\infty} \frac{k}{n} = E\left(\Psi_i\right). \tag{2.107}$$

where $E\left(\Psi_i\right) = S\left(\hat{\rho}_A\right) = S\left(\hat{\rho}_B\right)$ is the so-called entanglement entropy, given by the von Neumann entropy of the reduced density matrix, $\hat{\rho}_{A(B)} = Tr_{B(A)}\hat{\rho}_{AB}$, of the subsystems. The higher the entanglement of each $\left|\Psi_i\right\rangle_{AB}$, for $\theta \to \frac{\pi}{4}$, the higher the entropy $S\left(\hat{\rho}_A\right)$ gets and consequently the more singlets $m \to nS\left(\hat{\rho}_A\right)$ can be *distilled* from the initial state (2.105). This will be a key ingredient in Section 2.8, where we will talk about entanglement measures. Moreover, the converse statement is also true, i.e. given n shared singlets then via local operations and classical communication we can prepare m arbitrarily good copies of $\left|\Psi_i\right\rangle_{AB}$, with

$$\lim_{n\to\infty} \frac{k}{n} = \frac{1}{E\left(\Psi_i\right)}. \tag{2.108}$$

In plain words, the more entangled $\left|\Psi_i\right\rangle_{AB}$ is (i.e. high $E\left(\Psi_i\right)$), the more singlets are needed to prepare it. Note that these quantities are given meaning only asymptotically, in the limit of infinite copies n. A very useful quantity is the so-called *entanglement of formation* (E_F), defined as

$$E_F = \lim_{n\to\infty} \frac{k_{\min}}{n}, \tag{2.109}$$

which actually is the minimum value of (2.108). In other words, E_F gives us the minimum number k_{min} of singlets that are needed to prepare n copies of some given state. These results correspond, however, to the simple case in which the entangled state of the pairs (2.105) is pure. Let us see what happens in the more interesting, and general, case where the state $\hat{\rho}_{AB}$, of each pair, is mixed.

In another paper [52], Bennett *et. al.* considered the more general case, where the density matrix $\hat{\rho}$ of each of the n pairs is mixed,

$$\hat{\rho}\left(A,B\right) = \underbrace{\hat{\rho}\otimes\hat{\rho}\otimes\cdots\otimes\hat{\rho}}_{n}. \quad \left(Tr\hat{\rho} < 1\right) \tag{2.110}$$

They introduced a protocol, consisting of instructions about how Alice and Bob may coordinate the local manipulations of their qubits, so that in each step they are able to increase the, so-called, *fidelity* of $\hat{\rho}$ closer to one. The fidelity is defined as

$$F = \left\langle\psi^-\right|\hat{\rho}\left|\psi^-\right\rangle, \tag{2.111}$$

and, consequently, as $\hat{\rho}$ approaches the singlet $\left|\psi^-\right\rangle\left\langle\psi^-\right|$ the fidelity approaches unity, $F \to 1$. The new fidelity F', after completing a step of the protocol, is related to the previous fidelity F via the recurrence relation

$$F'\left(F\right) = \frac{F^2 + \frac{1}{9}\left(1-F\right)^2}{F^2 + \frac{2}{3}F\left(1-F\right) + \frac{5}{9}\left(1-F\right)^2}. \tag{2.112}$$

It can be shown that *only if* the initial fidelity of the state, $F = \left\langle\psi^-\right|\hat{\rho}\left|\psi^-\right\rangle$, satisfies $F > \frac{1}{2}$, F' may converge to 1 for sufficiently large number copies n of the initial state $\hat{\rho}$. In other words, the distillation protocol will work only for not-too-impure mixed states.

In contrast to the previous case, of the pure initial state, Bennett *et. al.* were not able to find the optimal value of

$$D\left(\hat{\rho}\right) = \lim_{n\to\infty} \frac{k_{\max}}{n}, \tag{2.113}$$

where $k_{\max}$ is the maximum number of singlets that can be distilled from the initial n state $\hat{\rho}$. This quantity, $D\left(\hat{\rho}\right)$, is known as *entanglement of distillation* and is also a measure of entanglement.

2.7.1 Bound Entanglement

We saw that it's possible to distil some pure entanglement out of a not maximally entangled and generally mixed state. But is this *always* possible? In [53], M. Horodecki *et. al.* showed that *any* inseparable mixed state of dimensions 2×2 can be distilled to a singlet form, no matter how mixed or whether its fidelity is small, i.e. $F \leq \frac{1}{2}$. In proving this result, they realised, that, in order for an entangled quantum state to be distilled it needs to violate the PPT criterion (see Sec. 2.6.2). But, remember, there are states of dimensions other than 2×2 and 2×3, that may be entangled and still not violate the PPT criterion. This fact led M. Horodecki *et. al.* to another paper [54], where they proved that any entangled quantum state, of *any* dimensions, can be distilled *if and only if* it violates the PPT criterion.

This is an important result because it proves that distillation totally depends on the PPT criterion and, furthermore, it shows that there are entangled states that cannot be distilled! These are those states that are entangled and do not violate the PPT criterion. An example of such a state is,

$$\hat{\rho}_{AB} = \frac{1}{8a+1} \begin{pmatrix} a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & 0 & 0 & 0 & 0 & 0 \\ a & 0 & 0 & 0 & a & 0 & 0 & 0 & a \\ 0 & 0 & 0 & 0 & 0 & a & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1+a}{2} & 0 & \frac{\sqrt{1-a^2}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 0 \\ a & 0 & 0 & 0 & a & 0 & \frac{\sqrt{1-a^2}}{2} & 0 & \frac{1+a}{2} \end{pmatrix}, \tag{2.114}$$

that describes two spin-1 particles, with Hilbert space dimension 3×3. This state was shown[55] to be entangled, via other criteria, and have a positive partial transpose at the same time; such a state cannot be distilled. Moreover, all the separable states are PPT and, as expected, no entanglement can be distilled from separable states.

We have reached the conclusion, that, there are two kinds of entanglement in nature. The *free* entanglement that can be distilled to a singlet form, being useful for quantum information tasks, and a *bound* entanglement that is not distillable.

For a thorough investigation of entanglement distillation and bound entanglement, see the Ph.D. thesis of L. Clarisse [56].

2.8 Entanglement Measures

We have now come to one of the most important topics in Quantum Information Theory, namely that of *entanglement measures.* The question that we want to explore is,

- *Can entanglement be quantified?*

It's not even clear that such a question has a meaning after all. A state can surely be either entangled or separable, but in what sense may we say that an entangled state is more entangled than another entangled state? As for an example, consider the following entangled states; the maximally entangled singlet

$$\left|\psi^{-}\right\rangle_{AB} = \frac{1}{\sqrt{2}}\left(\left|10\right\rangle_{AB} - \left|01\right\rangle_{AB}\right), \tag{2.115}$$

and a not-maximally entangled state,

$$\left|\Psi\right\rangle_{AB} = \cos\theta\ \left|10\right\rangle_{AB} + \sin\theta\ \left|01\right\rangle_{AB}. \tag{2.116}$$

They are both entangled (for $\theta \neq 0, \pi$), and they both have Schmidt number 2, a number which cannot increase via local operations, so why would we consider $\left|\Psi\right\rangle_{AB}$ less entangled than $\left|\psi^{-}\right\rangle_{AB}$? There are two popular and different approaches to this problem, the operational and the axiomatic approach.

The *operational approach* was initiated by Bennett *et. al.*[57],[58], and it's based on how efficient an entangled state is for a given quantum information task that would, else, be impossible without entanglement. Such tasks, for example, are the teleportation of quantum states, violating Bell's inequalities (useful in quantum cryptography), quantum super-dense coding etc. In these kind of tasks, the Bell states, like the singlet (2.115), show the maximum efficiency and that's why we call them maximally entangled states. Entangled states like (2.116), or more general mixed entangled states, are not so efficient in these tasks. For example, they cannot teleport a quantum state faithfully or cannot violate Bell's inequality as much as the singlet, or violate at all for many mixed entangled states.

Realizing that the Bell states, like the singlet, are maximally entangled in the operational sense that we just described, is the key ingredient in our search of how to quantify the entanglement of general states. As we have discussed, quantum entanglement cannot be created by via local operations (LOCC), the latter can only conserve it or destroy it. The idea is to use local operations to convert a given quantum state $\hat{\rho}$ to a common currency, e.g. a singlet state, that operates best in quantum information tasks. This conversion was discussed in Section 2.7 on entanglement distillation/concentration. So, given n copies for each of the two entangled states $\hat{\rho}_1$, $\hat{\rho}_2$, we convert both via LOCC into singlets. The state that is more entangled is defined to be the one that has been converted to a larger number of singlets and, hence, will more more useful in quantum information tasks. Some examples of various entanglement measures are the following:

• *Entanglement of Distillation:* It's defined as the maximum number k_{max} of singlets that can be, approximately, extracted from n copies of some bipartite state $\hat{\rho}$ via some LOCC procedure,

$$E_D\left[\hat{\rho}\right] = \lim_{n\to\infty}\ \frac{k_{\max}}{n} = \sup_{LOCC}\ \lim_{n\to\infty}\ \frac{k}{n}. \tag{2.117}$$

It's evident that $0 \leq E_D[\hat{\rho}] \leq 1$, and the higher $E_D[\hat{\rho}]$ is the more entangled $\hat{\rho}$ is considered to be. Here, $\sup_{LOCC}$ denotes the maximization over all possible LOCC protocols that fulfil the desired distillation, making the calculation a very difficult task. In the case when $\hat{\rho}$ is pure, $E_D[\hat{\rho}]$ is equal to the *entropy of entanglement* defined as the von Neumann entropy of the reduced state of the subsystems,

$$E_D[\hat{\rho}_{AB}] = E[\hat{\rho}_{AB}] = S(\hat{\rho}_A). \tag{2.118}$$

We remind that the von Neumann entropy of some state $\hat{\rho}$ is defined as $S(\hat{\rho}) = -Tr(\hat{\rho}\log\hat{\rho})$, for a more detailed discussion on this see [5].

• *Entanglement of Formation:* It's defined as the minimum number k_{min} of singlets needed to create (or form, hence the name formation) n copies of some state $\hat{\rho}$,

$$E_F[\hat{\rho}] = \lim_{n\to\infty} \frac{k_{\min}}{n} = \inf_{LOCC} \lim_{n\to\infty} \frac{k}{n}, \tag{2.119}$$

where $\inf_{LOCC}$ denotes the minimization over all possible LOCC protocols. It's domain is $0 \leq E_F[\hat{\rho}] \leq 1$, and the higher $E_F[\hat{\rho}]$ is, the more singlets are needed to construct $\hat{\rho}$, hence the more entangled $\hat{\rho}$ is considered to be. This entanglement measure is also important in an operational sense, but, as the entanglement of distillation, it's very difficult to compute due to the required minimization over all LOCC protocols. However, recent progress was due to W. Wooters [97], who was able to find a closed analytical form of E_F in the special case of bipartite qubit states, valid for any mixedness. Wooters defined another quantity, named *concurrence*, and proved that it's analytically connected to E_F in the aforementioned special case. We will analyse this quantity more in the subsequent sections, together with another popular measure, the *negativity*, due their practical importance. Finally, let us mention, that, for pure states the following equality can be proved[7],

$$E_D = E_F = E. \tag{2.120}$$

Another approach was initiated by V. Vedral *et. al.* [59], known as the *axiomatic approach*. They introduced the idea that any function satisfying some basic postulates could be regarded as an entanglement measure. The most important of postulates is,

◦ *Monotonicity under LOCC*: Indeed, we know that entanglement cannot be created by local operations and communication, consequently no entanglement measure should be increased after any LOCC operation. If we denote as Λ the action of a LOCC operation, any entanglement measure E should satisfy

$$E[\Lambda(\hat{\rho})] \leq \mathrm{E}[\hat{\rho}]. \tag{2.121}$$

For the general form of LOCC operations, $\Lambda(\hat{\rho})$, see [59].

◦ *Vanishing on separable states*: By definition, separable states have no entanglement, hence an entanglement measure should equal a constant minimum value C for all separable states,

$$\mathrm{E}[\hat{\rho}_{sep}] = c, \quad \forall\hat{\rho}_{sep}, \tag{2.122}$$

and it's natural to set $c = 0$.

These two are the most basic postulates, and perhaps the only ones, that all entanglement measures should satisfy. There are various other postulates that may be introduced, for a more detailed overview see [3], [60]. In the next two sections, we will analyse two important entanglement measures, the aforementioned *concurrence* and *negativity* due to their high practical importance, and their use in Part III of the Thesis.

2.8.1 Concurrence

The various entanglement measures that we previously discussed, though very important, are very difficult to be calculated analytically, due to the minimization/maximization condition over all LOCC operations. So, practically E_D and E_F as given by (2.118) and (2.119), respectively, are just formal expressions. The first successful attempt towards an easily computable entanglement measure was due to W. K. Wootters [97], who derived an analytical formula for the entanglement of formation E_F of an arbitrary state of two qubits, which he expressed via another quantity named *Concurrence*. In particular, he showed that for a general state of two qubits it holds,

$$E_F(C) = H\left(\frac{1+\sqrt{1-C^2}}{2}\right), \tag{2.123}$$

where C is the concurrence, and $H(x)$ is the so-called Shannon entropy defined as,

$$H(x) = -x\log_2 x - (1-x)\log_2(1-x). \tag{2.124}$$

As we know, and as can be seen from (2.123), $E_F(C)$ is bounded by

$$0 \leq E_F(C) \leq 1, \tag{2.125}$$

and it's monotonically increasing from 0 to 1 as C goes from 0 to 1. In this sense, C acquires the meaning of an entanglement measure by itself and can be used instead of E_F. Let us now see how to actually compute the concurrence C.

The concurrence is based on the "spin flip" transformation, which for a bipartite state $\hat{\rho}$ reads

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\,\rho^*\,(\sigma_y \otimes \sigma_y), \tag{2.126}$$

where the Paul matrices flip the spin of each qubit, and is equivalent to the time reversal operation. With ρ^* we denote the complex conjugate of the state when expressed in the standard basis $\{|\uparrow_z\uparrow_z\rangle,\ |\downarrow_z\downarrow_z\rangle,\ |\uparrow_z\downarrow_z\rangle,\ |\downarrow_z\uparrow_z\rangle\}$. Having defined the spin-flipped density matrix, the desired formula for the concurrence reads

$$C(\rho) = \max\left\{0, \sqrt{R_1} - \sqrt{R_2} - \sqrt{R_3} - \sqrt{R_4}\right\}, \tag{2.127}$$

where the $R_i s$ are the decreasingly ordered eigenvalues of the matrix

$$\begin{aligned} R &\equiv \rho\tilde{\rho} \\ &= \rho\,(\sigma_y \otimes \sigma_y)\,\rho^*\,(\sigma_y \otimes \sigma_y). \end{aligned} \tag{2.128}$$

Intuitively we understand why C detects entanglement, since the operation (2.127) reminds us of the partial transpose operation employed in the PPT criterion, which is also related to the time reversal. Ofcourse, in order to prove that C is actually an entanglement measure, and that is connected with E_F via an analytical formula, is a more tedious task. Concurrence was first discovered by Hill and Wootters in [96], but only for some special states. The important generalization to all bipartite states was proven by Wootters in [97]. After introducing the next important computable measure, the *negativity*, we will work out a specific example to see these entanglement measures in action, together with their interplay.

2.8.2 Negativity

Emphasizing, again, the importance of having a practical entanglement measure that can be easily computed, we are faced with a serious gap in the literature. Without even mentioning multipartite entanglement with more than two qubits, we find that they are is no easily computable entanglement measure even for the *simple* bipartite scenario. The only exception is the aforementioned *concurrence* of Wootters but, still, it works only for *qubit* states. What about bipartite sytems of higher dimensions, like 2×3 or $d_1 \times d_2$ in general? This gap was partially filled by Vidal and Werner in [95], by introducing *Negativity*. We say "partially" because this measure doesn't always detect entanglement for states with dimension higher than 2×3, in particular it cannot detect the PPT entangled states (that doesn't violate the PPT criterion). Let us examine this measure in more detail though.

This entanglement measure is based on Peres' PPT criterion, which we examined in detail in Section 2.6.2. We saw that if a bipartite density matrix $\hat{\rho}$ is entangled, then its partial transpose $\hat{\rho}^{PT}$ may have negative eigenvalues, which we denote as λ_i. *Negativity* is now defined as,

$$N(\rho) = \left| \sum_i \lambda_i \right| . \tag{2.129}$$

This expression is intuitive, in the sense that only the entangled states have $\lambda_i \neq 0$, and when an entangled state approaches (approximately) a separable state then $\lambda_i \to 0$ and the measure N is vanishes. Consequently, the "further away" an entangled state is from a separable state, the higher its λ_i, hence N, will be. Moreover, the eigenvalues λ_i are easily calculable, making N a very practical measure. Although (2.129) seems to be a natural choice, we need to see, for example, if it satisfies the various postulates that we introduced in this section -postulates that every entanglement measure should satisfy- plus, if it has any operational meaning as well.

In [95], Vidal and Werner proved the following properties of negativity,

Properties of Negativity

- $N(\rho)$ *is an entanglement monotone*, i.e. it does not increase under *LOCC*,

$$N(\Lambda[\rho]) \leq N(\rho), \tag{2.130}$$

  where Λ denotes a general LOCC operation.

- $N(\rho)$ *vanishes for all separable states*,

$$N(\rho_{sep}) = 0, \quad \forall \rho_{sep}. \tag{2.131}$$

That's natural, since all separable states satisfy the PPT criterion and, hence, their partial transpose has no negative eigenvalues.

- $N(\rho)$ *provides an explicit lower bound on how close* ρ *can be taken, by means of LOCC, to the maximally entangled state* $|\varphi^+\rangle$.

- $N(\rho)$ *provides an upper bound to teleportation capacity*, i.e. the ability of ρ to faithfully teleport a quantum state.

- $N(\rho)$ *provides an upper bound to the entanglement of distillation* E_D, i.e.

$$E_D(\rho) \leq E_N(\rho), \tag{2.132}$$

where the quantity

$$E_N(\rho) \equiv \log_2(1 + 2N(\rho)), \tag{2.133}$$

is known as *logarithmic negativity*. For separable states it's obvious that $E_D(\rho_{sep}) = 0$, due to $N(\rho) = 0$.

We see, that, *negativity* satisfies all the basic postulates that the axiomatic approach of entanglement measures imposes. Moreover, it also has an operational meaning due to the bounds on the teleportation capacity and distillation rate. In the next section we will work out a specific example, to see this measure, together with concurrence, in action. Ofcourse, our main application will be presented in *Part* IV.

2.8.3 An illustrative example

It is time that we illustrate the various aspects of bipartite entanglement and, also, see the two most important entanglement measures, $C(\rho)$ and $N(\rho)$ in action. The reader should consider this application as a warm-up for what's coming in Part III, where we will study more complex systems.

Consider two localized particles in space, named 1 and 2, depicted in Figure 2.5 as two red localized balls separated by some (arbitrary) distance. Both of these two particles have spin-$\frac{1}{2}$, and their spin degrees of freedom are entangled in a singlet state,

$$\left|\psi^-\right\rangle_{12} = \frac{1}{\sqrt{2}}\left(|01\rangle_{12} - |10\rangle_{12}\right). \tag{2.134}$$

This entanglement was, perhaps, created some time ago when these particles were together and interacted. We don't care how this entanglement came up, just that it exists. Two other localized spin-$\frac{1}{2}$ particles L and R, depicted as orange balls, are initially in the product state

$$|00\rangle_{LR} \equiv |0\rangle_L \otimes |0\rangle_R, \tag{2.135}$$

and, consequently, the initial state of the composite system of the four particles is,

$$|\varphi(0)\rangle = \left|\psi^-\right\rangle_{12} \otimes |00\rangle_{LR}. \tag{2.136}$$

Note that $\{|0\rangle, |1\rangle\}$ is the basis of definite spin in the z-direction, i.e. they are the eigenstates of σ_z. The orange particles approach the red particles and interact with them, for some time τ, via the spin-spin (Heisenberg) interaction Hamiltonian

$$H_{\text{int}} = H_{1L} + H_{2R}, \tag{2.137}$$

where,

$$H_{ij} = J\left(\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j\right), \tag{2.138}$$

with $i = 1, 2$ denoting the spins of the red particles, and $j = L, R$ the spins of the orange particles. H_{1L} is the interaction between the red particle 1 and the orange particle 2, and respectively for H_{2R}. The parameter J is the interaction's strength, which we assume to be constant throughout the duration of the interaction. Notice that the interacting pairs (1,L) and (2,R) are not interacting with each other, they could even be in causally disconnected regions of space-time. The time evolved quantum state of the four particles, after the interaction of duration τ, will be

$$\begin{aligned}
|\varphi(\tau)\rangle &= e^{-i\hat{H}_{\text{int}}\tau} |\varphi(0)\rangle \\
&= e^{-i\hat{H}_{1L}\tau} e^{-i\hat{H}_{2R}\tau} \left|\psi^-\right\rangle_{12} \otimes |00\rangle_{LR} \\
&= \frac{1}{\sqrt{2}} \left[\left(e^{-i\hat{H}_{1L}\tau}|00\rangle_{1L}\right) \otimes \left(e^{-i\hat{H}_{2R}\tau}|10\rangle_{2R}\right) - \left(e^{-i\hat{H}_{1L}\tau}|10\rangle_{1L}\right) \otimes \left(e^{-i\hat{H}_{2R}\tau}|00\rangle_{2R}\right)\right].
\end{aligned} \tag{2.139}$$

since $\left[\hat{H}_{1L}, \hat{H}_{2R}\right] = 0$. In order to make the calculations easier, we will express the Hamiltonians H_{ij} (2.138) through the ladder operators

$$\sigma_+ = \sigma_x + i\sigma_y, \quad \sigma_- = \sigma_x - i\sigma_y, \tag{2.140}$$

that satisfy the commutation relations

$$[\sigma_z, \sigma_\pm] = \pm\sigma_\pm. \tag{2.141}$$

The operator σ_+ raises the spin in the z-direction, while σ_- lowers it,

$$\sigma_+ |0\rangle = 2|1\rangle, \quad \sigma_- |1\rangle = 2|0\rangle \tag{2.142}$$

$$\sigma_+ |1\rangle = 0, \quad \sigma_- |0\rangle = 0. \tag{2.143}$$

The factor 2 is due to the fact, that, the Pauli operators are related to the spin operators via $S_\pm = \frac{\sigma_\pm}{2}$. Using these relations, we express H_{ij} as

$$\begin{aligned}
H_{ij} &= J\left(\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j\right) \\
&= J\left[\frac{1}{4}\left(\sigma_+^i + \sigma_-^i\right)\left(\sigma_+^j + \sigma_-^j\right) - \frac{1}{4}\left(\sigma_+^i - \sigma_-^i\right)\left(\sigma_+^j - \sigma_-^j\right)\right] \\
&= \frac{J}{2}\left(\sigma_+^i \sigma_-^j + \sigma_-^i \sigma_+^j\right).
\end{aligned} \tag{2.144}$$

In the next step, we must find how the exponentials $e^{-iH_{ij}\tau}$ act on the states. For this reason we Taylor expand them,

$$e^{-iH_{ij}\tau} = \sum_{n=0}^{\infty} \frac{(-i\tau H_{ij})^n}{n!} = \sum_{k=0}^{\infty} \frac{(-i\tau H_{ij})^{2k}}{(2k)!} + \sum_{k=0}^{\infty} \frac{(-i\tau H_{ij})^{2k+1}}{(2k+1)!}. \tag{2.145}$$

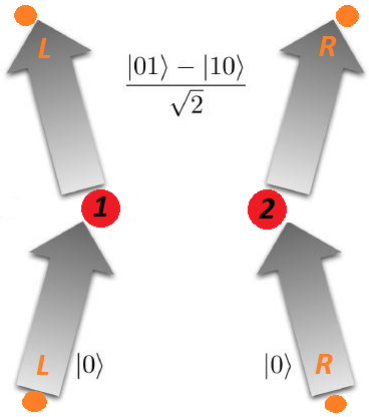

Figure 2.5: Each of the two spin-$\frac{1}{2}$ particles, L and R, depicted as orange balls, interact via a Heisenberg interaction with two other, entangled, particles 1 and 2, pictured as two red balls. After the interaction, the particles L and R exit in an entangled state, even though they never interacted directly. Last but not least, the distance between the particles 1 and 2 can be arbitrarily large, so here we witness the generation of entanglement between particles separated by a space-like distance.

We use this expansion to find the act of the exponential,

$$\bullet \quad H_{ij}|00\rangle_{ij} = \frac{J}{2}\left(\sigma_+^i\sigma_-^j + \sigma_-^i\sigma_+^j\right)|00\rangle_{ij} = 0 \tag{2.146}$$

$$\Rightarrow e^{-iH_{ij}\tau}|00\rangle_{ij} = e^0|00\rangle_{ij} = |00\rangle_{ij}, \tag{2.147}$$

$$\bullet \quad H_{ij}|00\rangle_{ij} = \frac{J}{2}\left(\sigma_+^i\sigma_-^j + \sigma_-^i\sigma_+^j\right)|00\rangle_{ij} = 0 \tag{2.148}$$

$$\Rightarrow e^{-iH_{ij}\tau}|11\rangle_{ij} = |11\rangle_{ij}, \tag{2.149}$$

$$\begin{aligned}\bullet \quad H_{ij}|01\rangle_{ij} &= \frac{J}{2}\left(\sigma_+^i|0\rangle_i \otimes \sigma_-^j|1\rangle_j + \sigma_-^i|0\rangle_i \otimes \sigma_+^j|1\rangle_j\right)\\ &= \frac{J}{2}\cdot 2|1\rangle_i \otimes 2|0\rangle_j\\ &= 2J|10\rangle_{ij},\end{aligned} \tag{2.150}$$

$$\begin{aligned}\Rightarrow \quad e^{-iH_{ij}\tau}|01\rangle_{ij} &= \sum_{k=0}^{\infty}\frac{(-i\tau)^{2k}}{(2k)!}\underbrace{H_{ij}^{2k}|01\rangle_{ij}}_{(2J)^{2k}|01\rangle_{ij}} + \sum_{k=0}^{\infty}\frac{(-i\tau)^{2k+1}}{(2k+1)!}\underbrace{H_{ij}^{2k+1}|01\rangle_{ij}}_{(2J)^{2k+1}|10\rangle_{ij}}\\ &= \left(\sum_{k=0}^{\infty}(-1)^k\frac{(2J\tau)^{2k}}{(2k)!}\right)|01\rangle_{ij} - i\left(\sum_{k=0}^{\infty}(-1)^k\frac{(2J\tau)^{2k+1}}{(2k+1)!}\right)|10\rangle_{ij}\\ &= \cos(2J\tau)\,|01\rangle_{ij} - i\sin(2J\tau)\,|10\rangle_{ij},\end{aligned} \tag{2.151}$$

and similarly,

$$\bullet \quad e^{-iH_{ij}\tau}|10\rangle_{ij} = \cos(2J\tau)\,|10\rangle_{ij} - i\sin(2J\tau)\,|01\rangle_{ij}. \tag{2.152}$$

We substitute the relations (2.147), (2.149), (2.151) and (2.152) in (2.139) and find the time-evolved quantum state,

$$|\varphi(\tau)\rangle = \cos(2J\tau)\ \ |00\rangle_{LR} \otimes \left|\psi^-\right\rangle_{12} - i\sin(2J\tau)\ \ \left|\psi^-\right\rangle_{LR} \otimes |00\rangle_{12}. \tag{2.153}$$

We see that for almost all times, the orange particles (L, R) have a non-zero possibility to exit the interaction in the maximally entangled singlet $|\psi^-\rangle_{LR}$, even though they never interacted. For the special times,

$$2J\tau = (2n+1)\frac{\pi}{2}, \quad n = 0, \pm1, \pm2, ... \tag{2.154}$$

the probability that this happens is one. So if we could control the interaction time, we would be able to create maximally entangled states. This process is known as *entanglement extraction*, since the entanglement of the orange particles (L, R) was extracted by the red particles $(1, 2)$. For more information on entanglement extraction, see *Part IV*. Let us now calculate the entanglement measures, negativity and concurrence, and see if they agree with these remarks.

Calculation of Concurrence .

The density matrix of the composite system of the four particles, after the interaction, is

$$\hat{\rho}_{LR12} = |\varphi(\tau)\rangle\langle\varphi(\tau)|. \tag{2.155}$$

Since we care about the entanglement of the orange particles (L, R), we compute their reduced density matrix,

$$\begin{aligned}\hat{\rho}_{LR} = Tr_{12}\hat{\rho}_{LR12} &= \sum_{i,j=0,1} {}_{12}\langle ij|\hat{\rho}_{LR12}|ij\rangle_{12} \\ &= \sin^2(2J\tau)\ \left|\psi^-\right\rangle_{LRLR}\left\langle\psi^-\right| + \cos^2(2J\tau)\ |00\rangle_{LRLR}\langle 00|.\end{aligned} \tag{2.156}$$

It's useful to work in the matrix form, so we consider the following representation,

$$\begin{gathered}|1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |0\rangle = \begin{pmatrix}0\\1\end{pmatrix} \\ |00\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}, \quad |11\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \\ |01\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \quad |10\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}.\end{gathered} \tag{2.157}$$

In this representation, the state $\hat{\rho}_{LR}$ takes the form

$$\hat{\rho}_{LR} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2}\sin^2(2J\tau) & -\frac{1}{2}\sin^2(2J\tau) & 0 \\ 0 & -\frac{1}{2}\sin^2(2J\tau) & \frac{1}{2}\sin^2(2J\tau) & 0 \\ 0 & 0 & 0 & \cos^2(2J\tau) \end{pmatrix}. \tag{2.158}$$

In order to calculate the concurrence, we define the matrix R (2.128),

$$\hat{R} = \hat{\rho}_{LR}\sigma_y \otimes \sigma_y \hat{\rho}^*_{LR}\sigma_y \otimes \sigma_y, \tag{2.159}$$

whose eigenvalues are

$$R_1 = \sin^4(2J\tau), \quad R_2 = R_3 = R_4 = 0. \tag{2.160}$$

Hence, the concurrence reads

$$\begin{aligned} C(\hat{\rho}_{LR}) &= \max\left\{0, \sqrt{R_1} - \sqrt{R_2} - \sqrt{R_3} - \sqrt{R_4}\right\} \\ &= \sin^2(2J\tau), \end{aligned} \tag{2.161}$$

and you can see in Figure 2.6 how C changes with time. Now notice something very interesting. If we made the same calculation of the concurrence but for the reduced state of the red particles $\hat{\rho}_{12}$, we would find

$$C(\hat{\rho}_{12}) = \cos^2(2J\tau). \tag{2.162}$$

Combining both, we find the following *entanglement conservation* relation

$$C(\hat{\rho}_{LR}) + C(\hat{\rho}_{12}) = 1, \quad \forall\tau. \tag{2.163}$$

The entanglement that the pair (L,R) extracts equals exactly the amount that the pair (1,2) lost. This a very peculiar characteristic of entanglement which is in pure contrast with classical correlation. The latter can be distributed between an arbitrary number of particles, while the amount of entanglement seems to be conserved between the particles. The laws that govern entanglement distribution were first explored by Coffman *et. al.* in [61] and this kind of behaviour is generally known as *monogamy of entanglement.* In its extremal form, it can be expressed as follows: If a qubit A is maximally entangled with a qubit B, then it cannot be entangled with a qubit C at the same time.

Calculation of Negativity .

In order to calculate the negativity $N(\hat{\rho}_{LR})$ we need the partially transposed state $\hat{\rho}^{PT}_{LR}$, which in matrix form is found to be

$$\hat{\rho}^{PT}_{LR} = \begin{pmatrix} 0 & 0 & 0 & -\frac{1}{2}\sin^2(2J\tau) \\ 0 & \frac{1}{2}\sin^2(2J\tau) & 0 & 0 \\ 0 & 0 & \frac{1}{2}\sin^2(2J\tau) & 0 \\ -\frac{1}{2}\sin^2(2J\tau) & 0 & 0 & \cos^2(2J\tau) \end{pmatrix}. \tag{2.164}$$

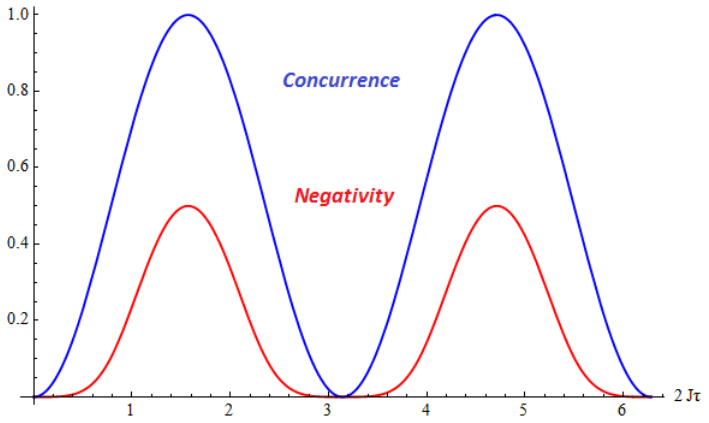

Figure 2.6: The concurrence $C\left(\hat{\rho}_{LR}\right)$ and negativity $N\left(\hat{\rho}_{LR}\right)$ of the orange particles is plotted, with respect to $2J\tau$. We notice the very similar behaviour of the measures, having their maxima and minima at the same interactions times.

Note that we have taken the partial transposition with respect to the subsystem R,

$$|01\rangle_{LRLR}\langle 10| \rightarrow |00\rangle_{LRLR}\langle 11|\,, \qquad |10\rangle_{LRLR}\langle 01| \rightarrow |11\rangle_{LRLR}\langle 00|\,. \tag{2.165}$$

The eigenvalues of the partially transposed state (2.164) are found to be,

$$\lambda_1 = \lambda_2 = \frac{1}{2}\sin^2\left(2J\tau\right) \geq 0, \quad \forall\tau \tag{2.166}$$

$$\lambda_3 = \frac{1}{4}\left(1+\cos^2\left(4J\tau\right)+\sqrt{3+\cos\left(8J\tau\right)}\right) \geq 0, \quad \forall\tau \tag{2.167}$$

$$\lambda_4 = \frac{1}{4}\left(1+\cos^2\left(4J\tau\right)-\sqrt{3+\cos\left(8J\tau\right)}\right) \leq 0, \quad \forall\tau. \tag{2.168}$$

Only λ_4 is negative, and it's negative for every τ. Hence, negativity (2.129) reads

$$\begin{aligned} N\left(\hat{\rho}_{LR}\right) &= |\lambda_4| \\ &= \frac{1}{4}\left|1+\cos^2\left(4J\tau\right)-\sqrt{3+\cos\left(8J\tau\right)}\right|. \end{aligned} \tag{2.169}$$

We have plotted negativity (2.169), together with concurrence (2.161), in Figure 2.6. They both agree with the way entanglement is distributed with time, by getting their maxima and minima at exactly the same interaction times. Moreover, the maxima happen for the interaction times (2.154), confirming the intuition that the pair (L,R) is maximally entangled at those times when they are described by the singlet state. For a complete review on quantum information with continuous variables, see [63].

Part III

Continuous-Variable Entanglement

Chapter 3

Basic formalism

In Part III, we will study Continuous-Variable (C.V.) entanglement which is present in many physical systems of interest, including photons, ions, BECs and even in one-particle systems. Therefore, due to the fact that the systems that we will study in the subsequent chapters are both discrete and continuous variable, it's customary to set out the necessary formalism for the latter. Last but not least, we talk about detecting C.V. entanglement by describing the most famous separability criteria, and, in the end, we will explore an idea of how to possibly improve these criteria. For reviews on the subject, see [62]-[65].

3.1 Second quantization formalism

In order to better understand continuous variable entanglement and, more importantly, spatial entanglement, we first need a basic understanding of the second quantization formalism which will help us define the spatial modes later on. A good reference of what we will discuss is [77].

In the second quantization formalism we work with the so-called occupation number states. Take for example N bosons in the following symmetrized state,

$$|n_1, n_2, \ldots\rangle = \left(\frac{n_1! n_2! \cdots}{N!}\right)^{1/2} \sum_{\text{permutations of } k_i} |k_1\rangle_1 \otimes |k_2\rangle_2 \otimes \cdots \otimes |k_N\rangle_N, \tag{3.1}$$

where the states $\{|k_i\rangle\}$ are the eigenstates of a one-particle operator corresponding to the particle j. For example, they could be the one-particle Hamiltonian's, H_j, eigenstates. The numbers n_i in the left hand side of (3.1) denote the number of particles in the corresponding eigenstate $|k_i\rangle$. For example, n_1 is the number of particles in the state $|k_1\rangle$, n_2 is the number of particles in the state $|k_2\rangle$ etc. Which means that some of the k_i, in the right hand side, could be equal -in order to have more than one particle in that state- so don't let the formalism confuse you just because the labelling is different. Since N is the total number of particles, it should hold

$$\sum_i n_i = N. \tag{3.2}$$

A general single-particle operator can be written as

$$\hat{F} = \sum_a \hat{f}_a, \tag{3.3}$$

where $\hat{f}_a$ acts on the Hilbert space H_a of particle a with orthonormal basis $\{|k_i\rangle_\alpha\}$. We know how such an operator acts on states $|k_i\rangle$, however since we want to work only with occupation number states like (3.1) we need to know exactly how the single particle operator $\hat{F}$ acts on them. After some algebra we find the following matrix elements[77],

$$\langle n_i, n_k - 1| \hat{F} |n_i - 1, n_k\rangle = {}_a\langle i| \hat{f}_a |k\rangle_a \sqrt{n_i n_k}. \tag{3.4}$$

Now we make the following observation. We can write the single-particle operator $\hat{F}$ in the form

$$\hat{F} = \sum_{i,j} {}_a\langle k_i| \hat{f}_a |k_j\rangle_a \hat{a}_i^\dagger \hat{a}_j, \tag{3.5}$$

where we have defined the ladder operators

$$\hat{a}_i |n_1, \ldots, n_i, \ldots\rangle = \sqrt{n_i} |n_1, \ldots, n_i - 1, \ldots\rangle, \tag{3.6}$$

with $\left[\hat{a}_i, \hat{a}_j^\dagger\right] = \delta_{ij}$ since it reproduces exactly the matrix elements (3.4). Notice that the operators $\hat{a}_i, \hat{a}_i^\dagger$ lower/raise the occupation number n_i of the single-particle state $|k_i\rangle$. The advantage of the form (3.5) is that we know exactly how this operator acts on the occupation number states since the ladder operators either destroy or create a particle in some state changing the corresponding number n_i by one. This is the so-called *second quantization formalism*. At this point we will not discuss where this nomenclature comes from since it's out of the scope of this Thesis. However note that the, differently written, form (3.5) is not so innocent as it looks, since the introduction of ladder operators gave us the ability to move from a Hilbert space of N particles to Hilbert spaces with different particle numbers. Mathematically, what we have done is to extend our mathematics and depart from the Hilbert space of N particles, i.e.

$$H^{N-particles} = H_1 \otimes \cdots \otimes H_N,$$

to the so-called *Fock space* defined as the direct sum of the, infinitely many, Hilbert spaces of different particle numbers, i.e.

$$H^{Fock} = H^{1-particle} \oplus \cdots \oplus H^{N-particles} \oplus \cdots \oplus H^{\infty-particles}.$$

Remarks and Discussion .

Now we would like to draw your attention to this very important point in order to understand what is to come. We defined some ladder operators $\{\hat{a}_i\}$ that lower/raise the occupation numbers of some states. But how can we define exactly what these states are? For example, we have seen in Quantum Field Theory that there are ladder operators that change the occupation number of momentum states, or position states, or angular momentum states etc. The action of the ladder operators is determined by the sandwich

$$\langle k_i| \hat{f}_a |k_j\rangle \tag{3.7}$$

in Eq. (3.5).

Whatever states $\{|k_i\rangle\}$ we wish to put in this sandwich, these states' occupation numbers will the ladder operators act on.

Example. Assume that $\{|p_i\rangle\}$ are momentum's eigenstates. Then by writing

$$\hat{F} = \sum_{i,j} {}_a\langle p_i|\, \hat{f}_a |p_i\rangle_a \hat{a}^\dagger_{p_i} \hat{a}_{p_j} \tag{3.8}$$

we have defined the action of $\hat{a}_{p_i}, \hat{a}^\dagger_{p_i}$ to lower/raise the occupation number of the single-particle momentum eigenstates $|p_i\rangle$, or ,in other words, they change the number of particles whose quantum state is $|p_i\rangle$. If we choose the operator $\hat{F}$ to be the total momentum operator, i.e.

$$\hat{P} = \sum_a \hat{p}_a, \tag{3.9}$$

where $\hat{p}_a$ where is the single-particle momentum operator of the particle a then it holds that

$${}_a\langle p_i|\, \hat{p}_a |p_j\rangle_a = p_i \delta_{ij}, \tag{3.10}$$

which makes (3.9) take the form

$$\hat{P} = \sum_i {}_a\langle p_i|\, \hat{p}_a |p_i\rangle_a \hat{a}^\dagger_{p_i} \hat{a}_{p_i} = \sum_i p_i \hat{a}^\dagger_{p_i} \hat{a}_{p_i}. \tag{3.11}$$

Since $\hat{a}^\dagger_{p_i} \hat{a}_{p_i}$ is the number operator whose eigenvalues are the number of particles with momentum p_i, we can see that $\hat{P}$ represents the total momentum in the system. We can do the same thing with the position operators, angular momentum, etc. Moreover, for every different index i we have an occupation of a different state, and it's customary to refer to these different operators $\hat{a}_{p_i}, \hat{a}^\dagger_{p_i}$ as *modes*.

At this point we would like to show one more thing which is also important. Since we can define different kinds of ladder operators, e.g. $\hat{a}_{p_i}, \hat{a}^\dagger_{p_i}$ that lower/raise the number of particles with momentum p_i or $\hat{a}_{x_i}, \hat{a}^\dagger_{x_i}$ that lower/raise the number of particles with position x_i, how are these different ladder operators related to each other? In order to show that, take the total momentum operator (3.9) and put in the sandwich 3.10 not momentum's eigenstates but position's eigenstates, i.e.

$$\hat{P} = \int dx \int dx' {}_a\langle x|\, \hat{p}_a |x'\rangle_a \hat{a}^\dagger_x \hat{a}_{x'}, \tag{3.12}$$

where the sum has been replaced by an integral due to the continuum of position. Next, we insert in the sandwich the spectral decomposition of unity to momentum eigenstates,

$$\begin{aligned}
\hat{P} &= \int dx \int dx' {}_a\langle x| \left(\sum_i |p_i\rangle_{aa} \langle p_i| \right) \hat{p}_a \left(\sum_j |p_j\rangle_{aa} \langle p_j| \right) |x'\rangle_a \hat{a}^\dagger_x \hat{a}_{x'} \\
&= \sum_{i,j} \langle p_i|\, \hat{p}_a\, |p_j\rangle \left(\int dx\, \langle x \mid p_i\rangle\, \hat{a}^\dagger_x \right) \left(\int dx'\, \langle p_j \mid x'\rangle\, \hat{a}_{x'} \right) \\
&= \sum_i p_i \hat{a}^\dagger_{p_i} \hat{a}_{p_i},
\end{aligned} \tag{3.13}$$

where we used (3.10) and, also, defined

$$\hat{a}_{p_i} = \int dx\, \langle p_i \mid x\rangle\, \hat{a}_x. \tag{3.14}$$

We showed how these different sets of ladder operators are related. We may have referred to the momentum and position operators but, since we didn't use this fact explicitely, the result (3.14) holds for any operators. This result is also of high importance for defining spatial entanglement later on, since we will need to be able to define ladder operators that lower/raise the occupation numbers of a localized wavefuction in the position space. For example, in the case where $\hat{P}$ above is the momentum operator, the destruction operator (3.14) destroys a particle with wavefunction $\langle x \mid p_i \rangle$. However this is not a localized wavefunction. On the other hand, if we choose a different single-particle operator $\hat{F}$ with localized eigenfunctions $|f_i\rangle$, in some region R, as eigenstates (e.g. the eigenfunction of a single particle Hamiltonian of an infinite square well are localized) then the ladder operator defined,

$$\hat{a}_{f_i}^{\dagger} = \int_R dx \, \langle x \mid f_i \rangle \, \hat{a}_x^{\dagger} = \int_R dx \, f_i(x) \, \hat{a}_x^{\dagger}, \tag{3.15}$$

creates a particle with wavefunction $f_i(x)$ non-zero only in the spatial region R. The important thing to grasp here is the following: In order for a ladder operator to create/destroy a localized particle, it should contain only those $\left\{\hat{a}_x, \hat{a}_x^{\dagger}\right\}$ with $x \in R$.

Once we have defined our desired ladder operators, e.g. $\hat{a}_p, \hat{a}_p^{\dagger}$, it's customary, in continuous variable treatments, to define the so-called phase space operators. That is, position- and momentum-like operators defined as

$$\hat{q}_p = \frac{1}{\sqrt{2}} \left(\hat{a}_p + \hat{a}_p^{\dagger}\right), \quad \hat{p}_p = \frac{-i}{\sqrt{2}} \left(\hat{a}_p - \hat{a}_p^{\dagger}\right), \tag{3.16}$$

satisfying the commutation relation $[\hat{q}_p, \hat{p}_p] = i$, hence their name. Of course, in general, these operators have absolutely nothing to do with the position and momentum of particle, like in harmonic oscillator systems, they just formally look the same. For example, in quantum optics, these operators are related with the observable electromagnetic field. Now, these observables (3.16) have continuous spectra, and their eigenstates, $|q\rangle$ and $|p\rangle$, belong to an *infinite* dimensional Fock space, since $q, p \in (-\infty, +\infty)$. Previously, we mentioned, that, the operators $\hat{a}_p, \hat{a}_p^{\dagger}$ for different index p correspond to different *modes*. When we will, later on, talk about entanglement in C.V. systems, we will refer to entanglement between the occupation number states of different modes. Since the observables of each mode have continuous spectra, we will call it *continuous variable entanglement.* Our goal will be to see how to detect such a C.V. entanglement, since its characteristics seem to be totally different from the discrete variable entanglement we discussed in *Part I.* It will be useful to study the C.V. systems in phase space, comprised of the aforementioned position- and momentum-like operators. In order to do that we will need some extra mathematical machinery, namely the distribution functions in phase space, such as the Wigner function and the characteristic function of a quantum state, which we will study in the next section.

3.2 Distribution functions in phase space and Gaussian states

The usage of phase space in quantum physics was initiated by Wigner, by introducing his infamous Wigner function [66], [67]. The Wigner function formalism is mathematically equivalent to the standard language of quantum mechanics. For simplicity, let us see how it's defined for a 1-mode system and for a pure state $|\Psi\rangle$,

$$\begin{aligned} W(q,p,t) &= \frac{1}{2\pi}\int \langle q-s/2,t|\left(|\Psi\rangle\langle\Psi|\right)|q+s/2,t\rangle\, e^{isp}ds \\ &= \frac{1}{2\pi}\int \langle p-s/2,t|\left(|\Psi\rangle\langle\Psi|\right)|p+s/2,t\rangle\, e^{isq}ds, \end{aligned} \tag{3.17}$$

where q and p are the eigenvalues of $\hat{q}$ and $\hat{p}$ respectively,

$$\hat{q}\,|q\rangle = q\,|q\rangle\,, \qquad \hat{p}\,|p\rangle = p\,|p\rangle\,. \tag{3.18}$$

This function satisfies some very important properties,

- $\int\int W(q,p,t)\,dqdp = 1,$ (3.19)
- $\int\int W(q,p,t)^2 dqdp = \frac{1}{2\pi},$ (3.20)
- $\rho(q,t) = |\Psi(q,t)|^2 = \int W(q,p,t)\,dp,$ (3.21)
- $\rho(p,t) = |\Psi(p,t)|^2 = \int W(q,p,t)\,dq,$ (3.22)
- $|\langle\Psi_1 \mid \Psi_2\rangle|^2 = 2\pi\int\int W_1(q,p,t)\,W_2(q,p,t)\,dqdp = \frac{1}{2\pi},$ (3.23)
- $\Psi(q,p,t) \to \Psi^*(q,p,t) \;\Rightarrow\; W(q,p,t) \to W(q,-p,t)\,,$ (3.24)
- $\Psi(q,p,t) \to \Psi(-q,p,t) \;\Rightarrow\; W(q,p,t) \to W(-q,-p,t)\,.$ (3.25)

It's obvious that the Wigner function $W(q,p,t)$ is a probability distribution, or, more accurately, a pseudo-probability distribution since it can be negative as well. The negativity of this function is a measure of the non-classicality of the given quantum state. A sufficient and necessary condition that $W(q,p,t)$ is strictly non-negative[68] is that $\Psi(q,p,t)$ is a Gaussian wave packet, having minimum uncertainty. We will define Gaussian functions in a while, right now let us generalize these expressions for a general n-mode, generally mixed, state $\hat{\rho}$. A compact way of writing such a *Wigner function* is the following,

$$\begin{aligned} W_\rho(X) &= \frac{1}{(2\pi)^n}\int\limits_{R^n} d^n s\;\; \langle\vec{q}-\vec{s}/2|\,\hat{\rho}\,|\vec{q}+\vec{s}/2\rangle\, e^{i\,\vec{s}\cdot\vec{p}} \\ &= \frac{1}{(2\pi)^{2n}}\int\limits_{R^{2n}} d^{2n}\Lambda\;\; \exp\left\{i\Lambda^{\mathrm{T}}\Omega X\right\}\chi_\rho(\Lambda)\,, \end{aligned} \tag{3.26}$$

where we have defined the real vectors $X = (x_1, y_1, \ldots, x_n, y_n)^T \in R^{2n}$, and $\Lambda = (a_1, b_1, \ldots, a_n, b_n)^T \in R^{2n}$, plus the so-called symplectic matrix given by

$$\Omega = \bigoplus_{k=1}^{n} \omega = \begin{pmatrix} \omega & & 0 \\ & \ddots & \\ 0 & & \omega \end{pmatrix}, \quad \text{where} \quad \omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{3.27}$$

The function $\chi_\rho(\Lambda)$ is known as, the *characteristic function* of the state $\hat{\rho}$, is given by

$$\chi_\rho(\Lambda) = Tr\left[\rho \ \exp\left\{-i\Lambda^{\mathrm{T}}\Omega\,\hat{R}\right\}\right], \tag{3.28}$$

where

$$\hat{R} = (\hat{q}_1, \hat{p}_1, \ldots, \hat{q}_n, \hat{p}_n)^T, \tag{3.29}$$

is a vector of operators, and particularly these operators $\hat{q}_i, \hat{p}_i$ are the modes (3.16). Since $[\hat{q}_i, \hat{p}_i] = i$, its matrix elements satisfy

$$\left[\hat{R}_i, \hat{R}_j\right] = i\Omega_{ij}, \tag{3.30}$$

where Ω is the matrix (3.27) defined above.

An important class of states in the continuum, are the *Gaussian states*. A single variable real function is called Gaussian when it has the form,

$$\Psi(x) \propto e^{ax^2+bx+c}, \tag{3.31}$$

where a, b, c are real constants, while for 2n-variables it generalizes to

$$\Psi(x_1, \ldots, x_n) \propto e^{a_1 {x_1}^2+b_1 x_1+c_1} \cdots e^{a_n {x_n}^2+b_n x_n+c_n} \tag{3.32}$$

There is another way of expressing (3.33) which is much more useful. It can be shown that this is equivalent to the following expression,

$$\Psi(x_1, \ldots, x_n) = \frac{\pi}{\sqrt{\det A}} e^{-\xi^T A\,\xi}, \tag{3.33}$$

where $\xi = (x_1, \ldots, x_n)^{\mathrm{T}}$, and A is a positive semi-definite matrix, containing real constants as matrix elements, and satisfy $\xi^{\mathrm{T}} A\,\xi \geq 0$ so that the function Ψ is normalizable to unity. Following this notation, the Wigner function is Gaussian if it can be brought in the form

$$W_\rho(X) = \frac{\exp\left\{-\frac{1}{2}\left(X - \left\langle \hat{R} \right\rangle\right)^T V^{-1} \left(X - \left\langle \hat{R} \right\rangle\right)\right\}}{\pi^n \sqrt{\det V}}, \tag{3.34}$$

where we defined the covariance matrix (CM)

$$V_{ij} = \frac{1}{2}\left\langle \left\{\Delta\hat{R}_i, \Delta\hat{R}_j\right\}\right\rangle = \frac{1}{2}\left\langle \hat{R}_i\hat{R}_j + \hat{R}_j\hat{R}_i\right\rangle - \left\langle \hat{R}_i\right\rangle\left\langle \hat{R}_j\right\rangle, \tag{3.35}$$

which is a positive semi-definite matrix, $X^T V X \geq 0$. The advantage of writing a Gaussian function in this form, is the explicit appearance of the calculable moments $\left\langle \hat{R}_i\right\rangle, \left\langle \hat{R}_i\hat{R}_j\right\rangle$,

instead of some unknown real constants. We can see that all these, up to second order, moments completely characterize a Gaussian state, and that will be a very important fact in entanglement detection. For a more complete treatment of these mathematical methods, see e.g. [69],[70].

As a final important note let us note the following. Notice from the definitions, that the density matrix, the Wigner function and the characteristic function are all related to each other via a proper Fourier transformation. As can be easily checked, a Fourier transformation preserves the Gaussian nature of a function. What this means is, that, if one of this functions is Gaussian, then the rest will be Gaussian as well. So, when we say that a quantum state is Gaussian, it means that all these functions are Gaussian in the representation (basis) of interest.

Chapter 4

Continuous-Variable Separability Criteria

After the necessary introductory material, we will discuss how to create entanglement criteria, in order to detect entanglement in a continuous-variable state. In contrast to Part II*, the dimension of Hilbert space is infinite, so it's not obvious how and if the PPT criterion will work in these dimensions. We will also see that Gaussian states play a special role in entanglement detection. In the subsequent sections we will present some of the most important entanglement criteria, apply them to some states and, finally, test a plausible idea on how to improve them.*

4.1 Simon's second-order criterion

R. Simon [82] used the PPT criterion, in the infinite dimensional Hilbert space, to derive separability criteria for bipartite states. The main idea will be to employ the partial transposition of the bipartite density matrix plus the uncertainty principle, however in the analysis we will use the covariance matrix (3.35) formalism which we will briefly explain.

In order not to let the reader get lost in the mathematical details, let us phrase the idea in simple words. Our starting point will be Schrodinger-Robertson[71] uncertainty principle for two observables $\hat{A}, \hat{B}$,

$$\sigma_A \sigma_B \geq \frac{1}{4}\left|\left\langle\left[\hat{A}, \hat{B}\right]\right\rangle_\rho\right|^2, \tag{4.1}$$

which is just a generalization of Heisenberg's for arbitrary observables $\hat{A}, \hat{B}$, or to be more precise, we will use the even more generalized uncertainty relation due to Dodonov, Kurmyshev and Man'ko [72],

$$\sigma_A \sigma_B - \sigma_{AB}^2 \geq \frac{1}{4}\left|\left\langle\left[\hat{A}, \hat{B}\right]\right\rangle_\rho\right|^2, \tag{4.2}$$

where we defined the (co)variances

$$\sigma_A = \left\langle\left(\Delta\hat{A}\right)^2\right\rangle = \left\langle\left(\hat{A} - \left\langle\hat{A}\right\rangle\right)^2\right\rangle = \left\langle\hat{A}^2\right\rangle - \left\langle\hat{A}\right\rangle^2, \tag{4.3}$$

$$\sigma_{AB} = \frac{1}{2}\left\langle \left\{ \Delta\hat{A}, \Delta\hat{B} \right\} \right\rangle = \frac{1}{2}\left\langle \hat{A}\hat{B} + \hat{B}\hat{A} \right\rangle - \left\langle \hat{A} \right\rangle \left\langle \hat{B} \right\rangle . \tag{4.4}$$

All the mean values are taken with respect to the density matrix of interest. The generalized version (4.2) gives us a better bound for the product of variances than Heisenberg's, if we have some knowledge about the state, i.e. if we know the covariance σ_{AB}.

Now, Simon's idea is based on the following fact. Suppose that the bipartite state $\hat{\rho}$ is entangled, then as we known from Section 2.6.2 the partial transposition of this state with respect to one of the subsystems, $\hat{\rho}^{PT}$, *may* lead to a non-physical density matrix with negative eigenvalues. This new, potentially non-physical, density matrix $\hat{\rho}^{PT}$ may even violate the fundamental uncertainty principle (4.2)! Consequently, Simon's criterion checks whether the uncertainty principle, taken with respect to the partially transposed state $\hat{\rho}^{PT}$, is violated or not. If it is violated, then entanglement has been detected.

Our first step to formally expressing Simon's criterion via the covariance matrix V, will be the following equivalence proved in [73],

$$\sigma_{x_i}\sigma_{p_i} - \sigma_{x_i p_i}^2 \geq \frac{1}{4} \quad \Leftrightarrow \quad V + \frac{i}{2}\Omega \geq 0, \tag{4.5}$$

where V is the covariance matrix of a bipartite system, defined in (3.35),

$$V_{ij} = \frac{1}{2}\left\langle \left\{ \Delta\hat{R}_i, \Delta\hat{R}_j \right\} \right\rangle = \frac{1}{2}\left\langle \hat{R}_i\hat{R}_j + \hat{R}_j\hat{R}_i \right\rangle - \left\langle \hat{R}_i \right\rangle \left\langle \hat{R}_j \right\rangle , \tag{4.6}$$

with

$$\hat{R} = \begin{pmatrix} \hat{q}_1 & \hat{p}_1 & \hat{q}_2 & \hat{p}_2 \end{pmatrix}^T, \tag{4.7}$$

and Ω is the symplectic matrix (3.27) for $n = 2$,

$$\Omega = \begin{pmatrix} \omega & 0 \\ 0 & \omega \end{pmatrix}, \quad \text{with} \quad \omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{4.8}$$

Moreover, the statement "$V + \frac{i}{2}\Omega \geq 0$" means that the 4×4 matrix $V + \frac{i}{2}\Omega$ is *positive semi-definite* and all of its eigenvalues are non-negative. Formally it's equivalent to the statement,

$$V + \frac{i}{2}\Omega \geq 0 \quad \Leftrightarrow \quad \xi\left(V + \frac{i}{2}\Omega\right)\xi^T \geq 0, \ \forall\xi. \tag{4.9}$$

We need a few more mathematical tools though. Say that we have been given the matrix V of some state $\hat{\rho}$, how can we know that the formed matrix "$V + \frac{i}{2}\Omega$" is positive semi-definite, hence the state satisfies the uncertainty principle? A first answer would be to find its eigenvalues and see whether they are non-negative. However, there is another, easier, way that doesn't require to diagonalize the matrix, and its based on Sylvester's criterion[74]. This criterion states that a symmetric non-singular matrix is positive semi-definite *if and only if* all of its *principal minors* are non-negative.

A principal minor of a square matrix, is defined as the determinant of that matrix, that you get if you delete the k^{th} row and k^{th} column of the initial matrix, while you may also delete multiple rows and columns, not just one. For example, the principal minors of the following 3×3 matrix

$$A = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{23} & \alpha_{33} \end{pmatrix}, \tag{4.10}$$

are

$$M_1 = \det\left[\begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{pmatrix}\right], \quad M_2 = \det\left[\begin{pmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{pmatrix}\right], \tag{4.11}$$

$$M_3 = \det\left[\begin{pmatrix} \alpha_{11} & \alpha_{13} \\ \alpha_{31} & \alpha_{33} \end{pmatrix}\right], \quad M_4 = \det\left[\begin{pmatrix} \alpha_{22} & \alpha_{23} \\ \alpha_{32} & \alpha_{33} \end{pmatrix}\right] \tag{4.12}$$

$$M_5 = \alpha_{11}, \quad M_6 = \alpha_{22}, \quad M_7 = \alpha_{33}. \tag{4.13}$$

Now if demand that A is positive semi-definite, i.e. $A \geq 0$, all of its principal minors should be non-negative,

$$M_i \geq 0, \quad \forall i. \tag{4.14}$$

The same should hold now for (4.5); if a state $\hat{\rho}^{PT}$ is physical, and hence satisfies the uncertainty principle, all the principal minors of the 4×4 matrix $\tilde{V} + \frac{i}{2}\Omega$ should be non-negative. First of all, we need to see how the covariance matrix $\tilde{V}$ of the partially transposed state $\hat{\rho}^{PT}$ is related to V of $\hat{\rho}$. Why? Because in the laboratory we can measure only the physical state $\hat{\rho}$, while $\hat{\rho}^{PT}$ is just an artificial artefact that needs to be expressed via something measurable. The covariance matrix $\tilde{V}$ is defined as,

$$\begin{aligned} \tilde{V}_{ij} &= \frac{1}{2}\left\langle \left\{ \Delta\hat{R}_i, \Delta\hat{R}_j \right\} \right\rangle = \frac{1}{2} Tr\left(\left\{ \Delta\hat{R}_i, \Delta\hat{R}_j \right\} \hat{\rho}^{PT} \right) \\ &= \int d^4R \; \Delta R_i \Delta R_j \, W_{\rho^{PT}}\left(q_1, p_1, q_2, p_2\right), \end{aligned} \tag{4.15}$$

where we expressed the mean values via the Wigner function (see [67] for details). Now let's calculate the Wigner function of $\hat{\rho}^{PT}$,

$$\begin{aligned} W_{\rho^{PT}}\left(q_1, p_1, q_2, p_2\right) &= \frac{1}{4\pi^2} \int d^2s \, \langle q_1 - s_1/2; q_2 - s_2/2 | \, \hat{\rho}^{PT} \, | q_1 + s_1/2; q_2 + s_2/2 \rangle \, e^{i(s_1 p_1 + s_2 p_2)} \\ &= \frac{1}{4\pi^2} \int d^2s \, \langle q_1 - s_1/2; q_2 + s_2/2 | \, \hat{\rho} \, | q_1 + s_1/2; q_2 - s_2/2 \rangle \, e^{i(s_1 p_1 + s_2 p_2)} \\ &= \frac{1}{4\pi^2} \int d^2s \, \langle q_1 - s_1/2; q_2 - s_2/2 | \, \hat{\rho} \, | q_1 + s_1/2; q_2 + s_2/2 \rangle \, e^{i(s_1 p_1 + s_2 (-p_2))} \\ &= W_\rho\left(q_1, p_1, q_2, -p_2\right), \end{aligned} \tag{4.16}$$

where at the last step we did a change of variables, $s_2 \to -s_2$. We have achieved to express the Wigner function of $\hat{\rho}^{PT}$ in terms of the Wigner function of $\hat{\rho}$, which is useful because our goal is to express $\tilde{V}_{ij}$ in terms of V_{ij}. Hence, due to (4.16), we have

$$\begin{aligned} \tilde{V}_{ij} &= \int d^4R \; \Delta R_i \Delta R_j \, W_{\hat{\rho}^{PT}}\left(q_1, p_1, q_2, p_2\right) \\ &= \int d^4R \; \Delta R_i \Delta R_j \, W_{\hat{\rho}}\left(q_1, p_1, q_2, -p_2\right). \end{aligned} \tag{4.17}$$

So, in order to go from V to $\tilde{V}$ we make the replacement $p_2 \to -p_2$,

$$\tilde{V} = V|_{p_2 \to -p_2} = \begin{pmatrix} V_{11} & V_{12} & V_{13} & -V_{14} \\ V_{12} & V_{22} & V_{23} & -V_{24} \\ V_{13} & V_{23} & V_{33} & -V_{34} \\ -V_{14} & -V_{24} & -V_{34} & V_{44} \end{pmatrix}. \tag{4.18}$$

Now we phrase Simon's separability criterion. If ρ^{PT} is a physical state, and hence $\hat{\rho}$ is separable, the following should be true

$$\sigma_{q_i}\sigma_{p_i} - \sigma_{q_i p_i}^2 \geq \frac{1}{4} \quad \Leftrightarrow \quad \tilde{V} + \frac{i}{2}\Omega \geq 0 \quad \Rightarrow \quad \det\left(\tilde{V} + \frac{i}{2}\Omega\right) \geq 0. \tag{4.19}$$

The third inequality corresponds to one of the principal minors being non-negative, and can be brought to the following convenient form

$$\begin{gathered} \det\left(\tilde{V} + \frac{i}{2}\Omega\right) \geq 0 \quad \Leftrightarrow \\ \det A \ \det B + \left(\frac{1}{4} - |\det C|\right)^2 - Tr\left[A\omega C\omega B\omega C^T J\right] \geq \frac{1}{4}\left(\det A + \det B\right), \end{gathered} \tag{4.20}$$

where the 2×2 matrices A, B, C are defined by $V = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix}$, and ω by (4.8). Eq. (4.20) is *Simon's criterion*. The violation of this inequality signals entanglement, while the non-violation of it tells us nothing about inseparability. It's interesting to write down the inequality for the uncertainty principle (4.19) as well,

$$\begin{gathered} \det\left(V + \frac{i}{2}\Omega\right) \geq 0 \quad \Leftrightarrow \\ \det A \ \det B + \left(\frac{1}{4} - \det C\right)^2 - Tr\left[A\omega C\omega B\omega C^T J\right] \geq \frac{1}{4}\left(\det A + \det B\right). \end{gathered} \tag{4.21}$$

As you can see, the only difference is the absence of the absolute value in $\det C$. Since the uncertainty principle (4.21) is *always* satisfied, and since the criterion (4.20) coincides the uncertainty principle (4.21) for $\det C > 0$, we conclude that the criterion can only be violated, hence detect entanglement, only for states with $\det C < 0$.

Simon proved another important result, however. He showed, that, if the quantum state $\hat{\rho}$ is Gaussian with respect to the local modes (4.7), having a Gaussian Wigner function of the form,

$$W_\rho(R) = \frac{\exp\left\{-\frac{1}{2}\left(R - \left\langle\hat{R}\right\rangle\right)^T V^{-1}\left(R - \left\langle\hat{R}\right\rangle\right)\right\}}{\pi^2\sqrt{\det V}}, \tag{4.22}$$

then Simon's criterion (4.22) is necessary and sufficient condition for separability. What this means is, that, if a Gaussian state satisfies the criterion then it's separable, but if it violates it it's entangled. For the majority of states, however, the non-Gaussian states, Simon's criterion doesn't always work, like Peres' criterion doesn't always work for Hilbert space dimensions higher than 2×3 in discrete variable systems. Gaussian states, on the other hand, is a very important class of states due to their experimental accessibility, hence this result is very important as well. This result on Guassian states should not come on surprise, since, as is obvious from (4.22), a Gaussian state is fully characterized by the covariance matrix of second-order moments. What this means is, that, if this state has any non-local correlations (due to entanglement), they will be present in the second

order moments and hence be detected by Simon's second order criterion. Non-Guassian states, on the other hand, cannot be described by their second order moments only but require moments up to infinite order in general. So, any non-local correlations could be present not in the second order moments but in higher orders, hence not detected by Simon's criterion.

Finally, let us comment on the special form (4.20) that we expressed the criterion, using only determinants and traces. Say that you have a quantum state $\hat{\rho}$ and want to see whether it's entangled or not. First things first, as we explained in Section 2.6.1, we first have to define exactly between what degrees of freedom are we searching for entanglement, or, in other words, we need to define a specific tensor product structure for the total Hilbert space. Say that we do that, e.g. $H_1 \otimes H_2$, we search for entanglement between the degrees of freedom belonging to Hilbert spaces H_1 and H_2 respectively. In order to do that, using Simon's criterion, we have to define position- and momentum-like observables for each Hilbert space (known as *local* observables), i.e.

$$\hat{q}_1, \hat{p}_1 \in H_1, \;\; \hat{q}_2, \hat{p}_2 \in H_2, \tag{4.23}$$

satisfying $[\hat{q}_i, \hat{p}_i] = i$. But the way that we can define these observables isn't uniquely defined. For example, instead of $\hat{q}_i, \hat{p}_i \in H_i$, we could also define

$$\hat{q}'_i = a\,\hat{q}_i + b\,\hat{p}_i \tag{4.24}$$

$$\hat{p}'_i = c\,\hat{q}_i + d\,\hat{p}_i, \tag{4.25}$$

with appropriate constants so that $[\hat{q}'_i, \hat{p}'_i] = i$ still holds. This transformation is linear (the new observables are linearly dependent on the initial ones) and canonical (preserves the commutation relation), and is known as a *symplectic transformation*. The most general of such transformations is to mix all the observables, and not just the local ones, known as *global* transformations. However, such transformations change our defined tensor product structure $H_1 \otimes H_2$, and hence are not considered. On the other hand, what we care about are the *local ones*, Eq. (4.24),(4.25). In matrix form, a general symplectic transformation S is defined as,

$$\hat{R} = \begin{pmatrix} \hat{q}_1 \\ \hat{p}_1 \\ \hat{q}_2 \\ \hat{p}_2 \end{pmatrix} \rightarrow \hat{R}' = \begin{pmatrix} \hat{q}'_1 \\ \hat{p}'_1 \\ \hat{q}'_2 \\ \hat{p}'_2 \end{pmatrix} = S \cdot \begin{pmatrix} \hat{q}_1 \\ \hat{p}_1 \\ \hat{q}_2 \\ \hat{p}_2 \end{pmatrix}, \text{ with } \left[\hat{R}'_i, \hat{R}'_j\right] = i\,\Omega_{ij}, \tag{4.26}$$

where $S \in Sp\,(4, R)$ is a real 4×4 matrix belonging to the symplectic group Sp of such matrices. The subgroup of the *local* canonical transformations, namely S_{local}, has the form

$$S_{local} = \begin{pmatrix} S_1 & 0 \\ 0 & S_2 \end{pmatrix} \in Sp\,(2, R) \otimes Sp\,(2, R) \subset Sp\,(4, R)\,. \tag{4.27}$$

Now we may answer our initial question, i.e. why the special form (4.20) using determinants and traces. Under arbitrary local transformations (4.28) of the modes, The matrices $V = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix}$ change as follows,

$$V \rightarrow SVS^T, \;\; A \rightarrow S_1 A S_1^T, \;\; B \rightarrow S_2 B S_2^T, \;\; C \rightarrow S_1 C S_2^T. \tag{4.28}$$

It can been shown, that, traces and determinants are invariant under these transformations, hence the criterion (4.20) keeps its form. What this also means is, that, the existence of entanglement does not depend on how you will choose the local modes, and that is an important result. But notice that this is not true for general transformations other than symplectic. For example, if we transform the initial modes via a general unitary transformation $\hat{U}$ that acts locally (not globally, staying in the same Hilbert space), i.e.

$$\hat{q}_i' = \hat{U}\hat{q}_i\hat{U}^T \neq a\hat{q}_i + b\hat{p}_i, \tag{4.29}$$

then Simon's criterion will not be invariant under such (local) transformations.

Example .

Let us see Simon's criterion in action using the following non-Gaussian two particle state,

$$\Psi_{\sigma_1,\sigma_2}(q_1,q_2) = N(q_1+q_2)\exp\left[-\frac{(q_1+q_2)^2}{4\sigma_2^2} - \frac{(q_1-q_2)^2}{4\sigma_1^2}\right], \tag{4.30}$$

where σ_1, σ_2 are real constants and

$$N = \frac{1}{\sqrt{\pi\sigma_1\sigma_2^3}}\sqrt{\frac{\sqrt{\sigma_1^2+\sigma_2^2}}{\sigma_1\sqrt{\frac{1}{\sigma_1^2}+\frac{1}{\sigma_2^2}}\sigma_2}}, \tag{4.31}$$

ensures the normalization of the state to unity,

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dq_1 dq_2 |\Psi_{\sigma_1,\sigma_2}(q_1,q_2)|^2 = 1. \tag{4.32}$$

This pure state can obviously *not* be written in a product form,

$$\Psi_{\sigma_1,\sigma_2}(q_1,q_2) \neq \chi(q_1)\cdot\varphi(q_2), \tag{4.33}$$

hence we can easily infer that it's an entangled state, for any value of σ_1, σ_2. But will Simon's criterion always be violated? The fact that this state is non-Gaussian makes the answer negative, i.e. Simon's criterion will not necessarily be violated, and we will see that this is true in the following calculations.

Our first task is to calculate all the covariance matrix elements V_{ij} (4.6). Let us calculate V_{14} in order to show how to do that. After noticing that the mean values of $\hat{q}_i, \hat{p}_i$ are zero in this state we have,

$$\begin{aligned} V_{14} &= \langle \hat{q}_1\hat{p}_2\rangle = \langle \Psi_{\sigma_1,\sigma_2}|\, \hat{q}_1\hat{p}_2\, |\Psi_{\sigma_1,\sigma_2}\rangle \\ &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dq_1 dq_2 \langle \Psi_{\sigma_1,\sigma_2} \mid q_1,q_2\rangle\, q_1 \left(-i\frac{\partial}{\partial q_2}\right)\langle q_1,q_2 \mid \Psi_{\sigma_1,\sigma_2}\rangle \\ &= -i\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dq_1 dq_2\, \Psi_{\sigma_1,\sigma_2}(q_1,q_2)\;\; q_1\frac{\partial\Psi_{\sigma_1,\sigma_2}(q_1,q_2)}{\partial q_2}, \end{aligned} \tag{4.34}$$

where we used the spectral decomposition of unity,

$$\hat{1} = \hat{1}_1 \otimes \hat{1}_2 = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dq_1 dq_2 \, |q_1\rangle_1 \otimes |q_2\rangle_2 \, {}_1\langle q_1| \otimes {}_2\langle q_2| \,, \tag{4.35}$$

and the representation of the momentum operator in position space,

$${}_2\langle q_2|\, \hat{p}_2 |q'{}_2\rangle_2 = -i\frac{\partial}{\partial q_2}\, \delta\left(q_2 - q'{}_2\right). \tag{4.36}$$

The calculation of (4.34) is now straightforward. We computed all the elements V_{ij} and the quantity

$$I_{Simon}\left(x\right) = \det A \;\det B + \left(\frac{1}{4} - \left|\det C\right|\right)^2 - Tr\left[A\omega C\omega B\omega C^T J\right] - \frac{1}{4}\left(\det A + \det B\right), \tag{4.37}$$

$$\text{where,} \quad x = \frac{\sigma_1}{\sigma_2}, \tag{4.38}$$

for various values of σ_1, σ_2, using *Mathematica* . A negative value, $I_{Simon} < 0$, will signal the existence of entanglement. We plotted $I_{Simon}\left(x\right)$ with respect to x in Figure 4.1, where we observe the violation of the criterion for all values of x, except in the region $0.58 \leq x \leq 1.75$, where $I_{Simon}\left(x\right) = 0$. We, indeed, observe what was expected. An entangled non-Gaussian state cannot always be detected by Simon's second order criterion.

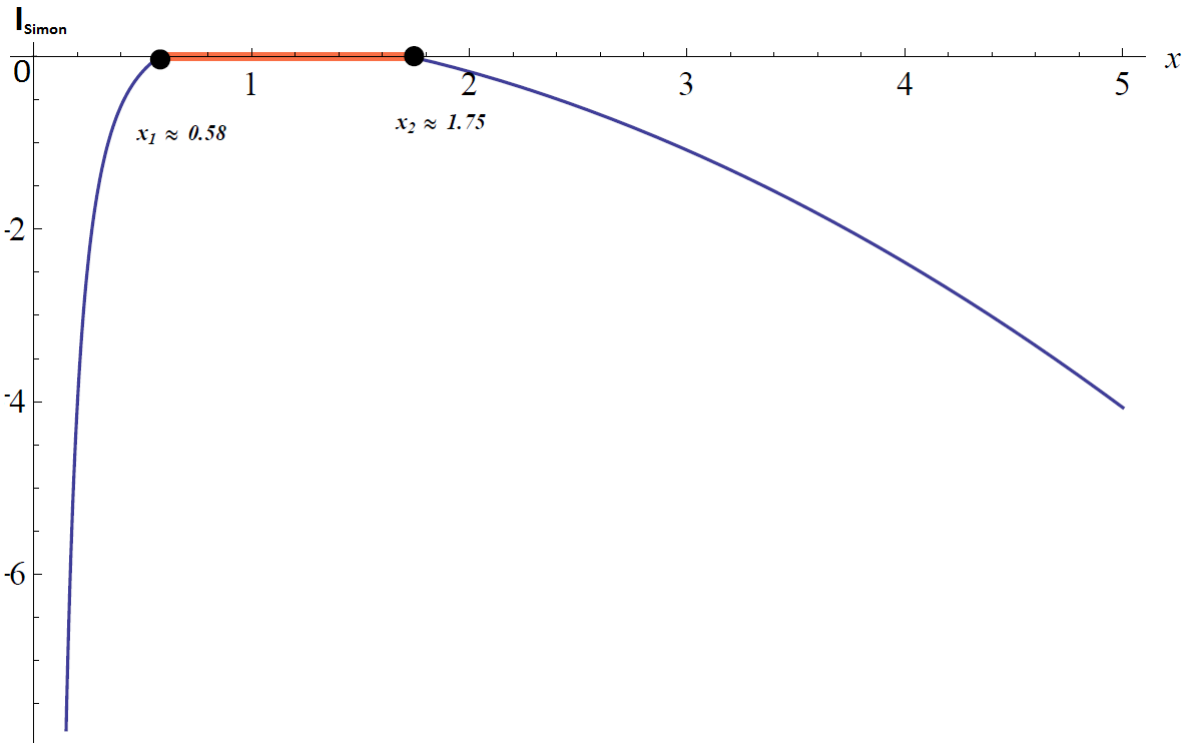

Figure 4.1: $I_{Simon}(x)$ is plotted for various values of $x = \frac{\sigma_1}{\sigma_2}$. The criterion is violated, $I_{Simon}(x) < 0$, for most values of x, except in the region $0.58 \leq x \leq 1.75$ denoted in red, where it's $I_{Simon}(x) = 0$. We see that Simon's criterion cannot always detect the entanglement of this pure bipartite non-Gaussian entangled state.

4.1.1 Can Simon's criterion be improved?

We saw that Simon's criterion doesn't always work for non-Gaussian states, because for some non-Gaussian states their corresponding partially transposed density matrix still satisfies the uncertainty principle (4.19), hence the criterion is not violated.

At this point, we would like to explore an idea. As we have repeatedly reported, Simon's criterion is equivalent to the uncertainty principle,

$$\sigma_{q_i}\sigma_{p_i} - \sigma^2_{q_ip_i} \geq \frac{1}{4}, \tag{4.39}$$

where q_i, p_i are the modes. Imagine that, instead of this inequality, we used another stronger uncertainty relation,

$$\sigma_{q_i}\sigma_{p_i} - \sigma^2_{q_ip_i} \geq \frac{1}{4}\Phi^2, \tag{4.40}$$

where Φ is function of either the global purity μ of the total bipartite state $\hat{\rho}$, i.e. $\Phi(\mu)$, or the von Neumann entropy S, i.e. $\Phi(S)$. As an example consider the first case, with the purity. This function always satisfies

$$\Phi(1) = 1 \leq \Phi(\mu) \leq \frac{1}{\mu}. \tag{4.41}$$

The more mixed the state is (low purity), the larger $\Phi(\mu)$ gets and, hence, the right hand side of this inequality (4.40) is generally larger than Heisenberg's $\frac{1}{4}$. It's only required that we, somehow, know the purity of the state in order to calculate the function $\Phi(\mu)$. Such uncertainty relations (4.40) have been developed [75], and are known as *bounded uncertainty relations*.

Now let's return to the exploration of a possible improvement. Assume that you have an entangled state $\hat{\rho}_{ent}$ with a corresponding partially transposed state $\hat{\rho}^{PT}_{ent}$. Suppose that we compute the uncertainty principle (4.39) with respect to $\hat{\rho}^{PT}_{ent}$ and find

$$\sigma_{q_i}\sigma_{p_i} - \sigma^2_{q_ip_i} = 1 \geq \frac{1}{4}, \tag{4.42}$$

not being violated. Now if the state was sufficiently mixed, and we knew the purity μ of $\hat{\rho}_{ent}$, then the use of the bounded uncertainty relation (4.40) could lead to a violation,

$$1 \leq \frac{1}{4}\Phi(\mu), \tag{4.43}$$

for sufficiently high $\Phi(\mu)$. Hence, we see that the exploitation of the bounded uncertainty relations could lead to a violation when the usual uncertainty relations do not, and this is the idea that we would like to explore.

The key point is to see how the uncertainty principle,

$$V + \frac{i}{2}\Omega \geq 0, \tag{4.44}$$

needs to be modified in the case of the bounded uncertainty relations (4.40). In order to do that, let us see how (4.44) is proved in the first place. In order to prove that the matrix

$V + \frac{i}{2}\Omega$ is positive semi-definite, we need to find its eigenvalues k_i and show that they are non-negative, $k_i \geq 0$. This we will do, by diagonalizing the matrix V using general symplectic transformations $S \in Sp\,(4, \Re)$. In fact, Williamson's theorem [76] guarantees the existence of such $S_W \in Sp\,(4, \Re)$, so that

$$V_W = S_W V S_W^T = \begin{pmatrix} \langle q_1'^2 \rangle & 0 & 0 & 0 \\ 0 & \langle p_1'^2 \rangle & 0 & 0 \\ 0 & 0 & \langle q_2'^2 \rangle & 0 \\ 0 & 0 & 0 & \langle p_2'^2 \rangle \end{pmatrix}, \tag{4.45}$$

with

$$\left\langle q_i'^2 \right\rangle = \left\langle p_i'^2 \right\rangle, \tag{4.46}$$

i.e. minimum uncertainty modes with zero covariance $\sigma_{q_i p_i} = 0$. where the transformed modes $\hat{q'}_i, \hat{p'}_i$ are connected with the old ones via (4.26) with $S = S_W$. Note that S_W is not a local transformation of the form $S_1 \otimes S_2$, but mixes the two modes. Since the symplectic transformations preserve the positive semi-definiteness of a matrix, hence its spectrum,

$$A \geq 0 \;\; \Leftrightarrow \;\; SAS^T \geq 0. \tag{4.47}$$

instead of finding the eigenvalues of $V + \frac{i}{2}\Omega$ we will equivalently find the eigenvalues of

$$S_W \left(V + \frac{i}{2}\Omega \right) S_W^T. \tag{4.48}$$

Taking advantage of the fact $S\Omega S^T = \Omega, \;\; \forall S$, we find

$$S_W \left(V + \frac{i}{2}\Omega \right) S_W^T = S_W V S_W^T + \frac{i}{2}\Omega = \begin{pmatrix} \langle q_1'^2 \rangle & \frac{i}{2} & 0 & 0 \\ -\frac{i}{2} & \langle p_1'^2 \rangle & 0 & 0 \\ 0 & 0 & \langle q_2'^2 \rangle & \frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & \langle p_2'^2 \rangle \end{pmatrix}. \tag{4.49}$$

The eigenvalues, k_i, of this matrix are now easily found to be

$$k_{i\pm} = \left\langle q_i'^2 \right\rangle \left\langle p_i'^2 \right\rangle \pm \frac{1}{4} \geq 0, \tag{4.50}$$

and are found to be always non-negative due to Heisenberg's uncertainty relation, hence the matrix $V + \frac{i}{2}\Omega$ is positive semi-definite as we already know. Thus it's always true that,

$$\det \left[V + \frac{i}{2}\Omega \right] = \left(\left\langle q_1'^2 \right\rangle^2 \left\langle p_1'^2 \right\rangle^2 - \frac{1}{16} \right) \left(\left\langle q_2'^2 \right\rangle^2 \left\langle p_2'^2 \right\rangle^2 - \frac{1}{16} \right) \geq 0. \tag{4.51}$$

The idea, now, is to improve this criterion by using the bounded uncertainty relations at the second step of the equality (4.51),

$$\left\langle q_i'^2 \right\rangle \left\langle p_i'^2 \right\rangle \geq \frac{1}{4}\Phi \left(\mu_i' \right) \geq \frac{1}{4}, \tag{4.52}$$

where $\mu_i^{'}$ is the reduced purity of the mode i of the transformed state corresponding to the diagonal covariance matrix (4.50). We could substitute (4.52) in (4.51) and get a stronger criterion,

$$\det\left[V+\frac{i}{2}\Omega\right] \geq \frac{1}{256}\left(\Phi^4\left(\mu_1^{'}\right)-1\right)\left(\Phi^4\left(\mu_2^{'}\right)-1\right). \tag{4.53}$$

However, there are two problems; first, we have to know the actual quantum state in order to be able to find what these reduced purities are and, also, the partial transposition that we should apply in order to get the criterion, may not generally preserve these purities. But even if the purities didn't change and we could write down the improved criterion, it would not be practical at all. All the second-order criteria are useful to experimentalists, since they contain moments only up to second order, hence they are easily measured experimentally. If we require that one should know the actual quantum state, this experimental convenience immediately vanishes, and there is no reason why to work with a second-order criterion in the first place, we could use higher order criteria like the ones we discuss in Section 4.3.

4.2 Duan *et. al.*'s second-order criterion

We saw that Simon took advantage of the PPT criterion, and used it for continuous variable systems as well, proving that it's necessary and sufficient for Gaussian states. At the same time, researchers from Innsbruck [83] -to call them Duan *et. al.*- were worried that the PPT criterion need not be sufficient when we move to the infinite dimensional Hilbert spaces, and constructed another well-known criterion based on the form that a separable density matrix takes.

The analysis is much simpler in this case. Just like with Simon's, we properly define the modes $\hat{q}_1, \hat{p}_1 \in H_1$ of the first subsystem and $\hat{q}_2, \hat{p}_2 \in H_2$ of the second subsystem. Next, we define the following observables,

$$\hat{u} = |a|\,\hat{q}_1 + \frac{1}{a}\hat{q}_2, \tag{4.54}$$

$$\hat{v} = |a|\,\hat{p}_1 - \frac{1}{a}\hat{p}_2, \tag{4.55}$$

where a is an arbitrary non-zero real constant. Suppose that we perform measurements on these observables; it's natural that if the quantum state $\hat{\rho}$ describing the two particles, is an eigenstate of these observables then our measurements would have zero variance, i.e.

$$\left\langle(\Delta\hat{u})^2\right\rangle_{\hat{\rho}} = \left\langle(\Delta\hat{v})^2\right\rangle_{\hat{\rho}} = 0, \tag{4.56}$$

since we would always find the same eigenvalue, while for any other states the variances will be non-zero,

$$\left\langle(\Delta\hat{u})^2\right\rangle_{\hat{\rho}} + \left\langle(\Delta\hat{v})^2\right\rangle_{\hat{\rho}} \neq 0. \tag{4.57}$$

We will prove, that, if state $\hat{\rho}$ is of separable form,

$$\hat{\rho}_{sep} = \sum_i p_i \hat{\rho}_{i1} \otimes \hat{\rho}_{i2}, \tag{4.58}$$

a lower bound is provided in the sum of variances (4.57) in terms of a. What this means is, that, the sum of variances of *every separable* state should be higher than this value, and only entangled states are allowed to go lower than this bound. So, experimentally we could make measurements and infer about the separability of the state without knowing what this state is, just like with Simon's criterion. This characteristic reminds us of the entanglement witnesses, discussed in Section 2.6.3, and indeed this is the case. These separability criteria can be viewed as entanglement witnesses. Now let's see what the aforementioned lower bound is for an arbitrary separable state of the form (4.58),

$$\begin{aligned}
\left\langle (\Delta\hat{u})^2 \right\rangle_{\hat{\rho}_{sep}} + \left\langle (\Delta\hat{v})^2 \right\rangle_{\hat{\rho}_{sep}} &= \sum_i p_i \left(\left\langle \hat{u}^2 \right\rangle_{\hat{\rho}_{i1}\otimes\hat{\rho}_{i2}\equiv\hat{\rho}_i} - \langle \hat{u} \rangle^2_{\hat{\rho}_i} \right) + \sum_i p_i \left(\left\langle \hat{v}^2 \right\rangle_{\hat{\rho}_i} - \langle \hat{v} \rangle^2_{\hat{\rho}_i} \right) \\
&= \sum_i p_i \left(a^2 \left\langle \hat{q}_1^2 \right\rangle_{\hat{\rho}_i} + \frac{1}{a^2} \left\langle \hat{q}_2^2 \right\rangle_{\hat{\rho}_i} + a^2 \left\langle \hat{p}_1^2 \right\rangle_{\hat{\rho}_i} + \frac{1}{a^2} \left\langle \hat{p}_2^2 \right\rangle_{\hat{\rho}_i} \right) + \\
&+ 2\frac{a}{|a|} \sum_i p_i \left(\langle \hat{q}_1 \rangle_{\hat{\rho}_i} \langle \hat{q}_2 \rangle_{\hat{\rho}_i} - \langle \hat{p}_1 \rangle_{\hat{\rho}_i} \langle \hat{p}_2 \rangle_{\hat{\rho}_i} \right) - \langle \hat{u} \rangle^2_{\hat{\rho}_{sep}} - \langle \hat{v} \rangle^2_{\hat{\rho}_{sep}} \\
= \sum_i p_i \Bigg[a^2 \underbrace{\left(\left\langle (\Delta\hat{q}_1)^2 \right\rangle_{\hat{\rho}_i} + \left\langle (\Delta\hat{p}_1)^2 \right\rangle_{\hat{\rho}_i} \right)}_{\geq 1} &+ \frac{1}{a^2} \underbrace{\left(\left\langle (\Delta\hat{p}_1)^2 \right\rangle_{\hat{\rho}_i} + \left\langle (\Delta\hat{p}_2)^2 \right\rangle_{\hat{\rho}_i} \right)}_{\geq 1} \Bigg] + \\
&+ \sum_i p_i \underbrace{\left(a^2 \langle \hat{q}_1 \rangle^2_{\hat{\rho}_i} + \frac{1}{a^2} \langle \hat{q}_2 \rangle^2_{\hat{\rho}_i} + 2\frac{a}{|a|} \langle \hat{q}_1 \rangle_{\hat{\rho}_i} \langle \hat{q}_2 \rangle_{\hat{\rho}_i} \right)}_{= \langle \hat{u} \rangle^2_{\hat{\rho}_i}} + \\
&+ \sum_i p_i \underbrace{\left(a^2 \langle \hat{p}_1 \rangle^2_{\hat{\rho}_i} + \frac{1}{a^2} \langle \hat{p}_2 \rangle^2_{\hat{\rho}_i} + 2\frac{a}{|a|} \langle \hat{p}_1 \rangle_{\hat{\rho}_i} \langle \hat{p}_2 \rangle_{\hat{\rho}_i} \right)}_{= \langle \hat{v} \rangle^2_{\hat{\rho}_i}} - \langle \hat{u} \rangle^2_{\hat{\rho}_{sep}} - \langle \hat{v} \rangle^2_{\hat{\rho}_{sep}} \\
&\geq a^2 + \frac{1}{a^2} + \left(\sum_i p_i \langle \hat{u} \rangle^2_{\hat{\rho}_i} - \langle \hat{u} \rangle^2_{\hat{\rho}_{sep}} \right) + \left(\sum_i p_i \langle \hat{v} \rangle^2_{\hat{\rho}_i} - \langle \hat{v} \rangle^2_{\hat{\rho}_{sep}} \right). \quad (4.59)
\end{aligned}$$

Note that in the third equality we used the uncertainty principle in the form of sums,

$$\left\langle \left(\Delta\hat{q}_j\right)^2 \right\rangle_{\hat{\rho}_i} + \left\langle \left(\Delta\hat{p}_j\right)^2 \right\rangle_{\hat{\rho}_i} \geq \left| \left[\hat{q}_j, \hat{p}_j \right] \right| = 1. \quad (4.60)$$

At the last step of (4.59) we will use Schwartz's inequality which says that,

$$\left| \sum_i x_i y_i^* \right|^2 \leq \sum_j |x_j|^2 \cdot \sum_k |y_k|^2, \quad (4.61)$$

for any set of complex numbers x_i, y_i. In our case, Schwartz's inequality is translated as,

$$\begin{aligned}
\langle \hat{u} \rangle^2_{\hat{\rho}_{sep}} = \sum_i \sqrt{p_i} \left(\sqrt{p_i} \langle \hat{u} \rangle_{\hat{\rho}_i} \right) \leq \underbrace{\sum_j \left| \sqrt{p_i} \right|^2}_{=1} \cdot \sum_j \left| \sqrt{p_i} \langle \hat{u} \rangle_{\hat{\rho}_i} \right|^2 = \sum_i p_i \langle \hat{u} \rangle^2_{\hat{\rho}_i} \;\Leftrightarrow \\
\sum_i p_i \langle \hat{u} \rangle^2_{\hat{\rho}_i} - \langle \hat{u} \rangle^2_{\hat{\rho}_{sep}} \geq 0.
\end{aligned} \quad (4.62)$$

Same for $\hat{v}$. Due to (4.62), Duan *et. al.*'s criterion (4.59) becomes,

$$\left\langle (\Delta\hat{u})^2 \right\rangle_{\hat{\rho}_{sep}} + \left\langle (\Delta\hat{v})^2 \right\rangle_{\hat{\rho}_{sep}} \geq a^2 + \frac{1}{a^2}. \tag{4.63}$$

Hence, only entangled states $\hat{\rho}_{ent}$ *may* violate this inequality,

$$0 \leq \left\langle (\Delta\hat{u})^2 \right\rangle_{\hat{\rho}_{ent}} + \left\langle (\Delta\hat{v})^2 \right\rangle_{\hat{\rho}_{ent}} < a^2 + \frac{1}{a^2}. \tag{4.64}$$

As Simon's, this as well is a second order criterion since it involves moments only up to second order. An important result that was also proved by Duan *et. al.* is, that, this criterion is also necessary and sufficient for Gaussian states, just like Simon's, but the constant a should be chosen equal to a specific value in this case. That is, this criterion is not necessary and sufficient (for Gaussian states) for just any value of a but the observables $\hat{u}, \hat{v}$ has to be chosen in the following specific way,

$$\hat{u} = a_0\,\hat{q}_1 - \frac{c_1}{|c_1|}\frac{1}{a_0}\hat{q}_2, \tag{4.65}$$

$$\hat{v} = a_0\,\hat{p}_1 - \frac{c_2}{|c_2|}\frac{1}{a_0}\hat{p}_2, \tag{4.66}$$

where $a_0^2 = \sqrt{\frac{m_1-1}{n_1-1}} = \sqrt{\frac{m_2-1}{n_2-1}}$. Now, let's see what are the constants m_i, n_i, c_i. We have seen that in (4.28) that under local, linear and canonical transformations (or, simply, symplectic transformations) the covariance matrix V of a state changes as

$$V \to SVS^T. \tag{4.67}$$

It can be proved [83] that there is always a transformation S_{II} such that V is transformed to the following standard form V_{II},

$$V = \begin{pmatrix} V_{11} & V_{12} & V_{13} & V_{14} \\ V_{12} & V_{22} & V_{23} & V_{24} \\ V_{13} & V_{23} & V_{33} & V_{34} \\ V_{14} & V_{24} & V_{34} & V_{44} \end{pmatrix} \to V_{II} = S_{II}VS_{II}^T = \begin{pmatrix} n_1 & 0 & c_1 & 0 \\ 0 & n_2 & 0 & c_2 \\ c_1 & 0 & m_1 & 0 \\ 0 & c_2 & 0 & m_2 \end{pmatrix}, \tag{4.68}$$

where you can see the desired constants m_i, n_i, c_i. How do we find this constants? Given a Gaussian quantum state, we calculate the covariance matrix (all its elements), and find the particular transformation S_{II} that brings it to the standard form V_{II}. Having done that, we read the constants from the V_{II}. As you see, unlike Simon's criterion, it's quite tedious to use Duan *et. al.*'s criterion for Gaussian states since we have to find the transformation S. This complication is due to the fact, that, this criterion is not invariant under symplectic transformations as Simon's, hence for every other Gaussian state, another transformation S is needed and the criterion's form changes. We will use Duan *et. al.*'s criterion together with Simon's, in *Part III*, to investigate the existence of entanglement in a non-Gaussian thermal state of great interest.

4.3 Shchukin and Vogel's generalized criteria

In the previous sections, we discussed the two most famous second-order separability criteria for bipartite continuous variables systems. These criteria are important mainly due to their experimental convenience; generally, the higher the moments $\left\langle \hat{q}_i^n \hat{p}_j^m \right\rangle$ we want to measure, the harder it is experimentally. So, the second order criteria is the least order at which entanglement can be detected (criteria of order one cannot detect entanglement), and it's experimentally the most feasible. On the other hand, higher-order criteria can also be derived which can be a lot more sensitive in entanglement detection than Simon's and Duan's. Shchukin and Vogel [84] developed a method via which entanglement criteria can be derived up to n order (with $n \to \infty$), with the criteria of Simon [82] and Duan *et. al.* [83], and other, to be just special cases of this more general approach.

Their idea is based on the PPT criterion plus the positivity of the density matrix. In order to see how it works, consider an arbitrary (generally not hermitian) operator $\hat{f}$ -that acts on the joint Hilbert space $H_1 \otimes H_2$- and construct the hermitian operator $\hat{f}^\dagger \hat{f}$. It's straightforward to see that for a legitimate bipartite density matrix $\hat{\rho}$, it holds that,

$$\left\langle \hat{f}^\dagger \hat{f} \right\rangle_{\hat{\rho}} = Tr\left(\hat{f}^\dagger \hat{f} \hat{\rho}\right) = \sum_n p_n \left\| \hat{f} \left| p_n \right\rangle \right\|^2 \geq 0, \quad \forall \hat{f}. \tag{4.69}$$

Employing now the PPT criterion, any separable state $\hat{\rho}$ satisfies

$$Tr\left(\hat{f}^\dagger \hat{f} \hat{\rho}^{PT}\right) \geq 0, \quad \forall \hat{f}, \tag{4.70}$$

since $\hat{\rho}^{PT}$ is a legitimate density matrix for separable states. Only entangled states are allowed to violate (4.70), hence this actually is the criterion. Now, the most general form of an arbitrary operator $\hat{f}$, that act on the occupation number states of the composite Hilbert space $H = H_1 \otimes H_2$, is[77]

$$\hat{f} = \sum_{n,m,k,l=0}^{\infty} c_{nkml}\, \hat{a}^{\dagger n} \hat{a}^m \hat{b}^{\dagger k} \hat{b}^l, \tag{4.71}$$

where $\hat{a}|n\rangle_1 = n|n-1\rangle_1 \in H_1$, $\hat{b}|n\rangle_2 = n|n-1\rangle_2 \in H_2$, and

$$c_{nmkl} = {}_1\langle n| \otimes {}_2\langle k|\ \hat{f}|m\rangle_1 \otimes |l\rangle_2 \equiv {}_{12}\langle nk|\, \hat{f}|ml\rangle_{12}. \tag{4.72}$$

Substituting (4.71) back to (4.70), we get

$$Tr\left(\hat{f}^\dagger \hat{f} \hat{\rho}^{PT}\right) = \sum_{n,k,m,l,p,q,r,s=0}^{\infty} c^*_{pqrs}\, c_{nmkl}\, M_{pqrs,nmkl} \geq 0, \quad \forall \hat{f} \tag{4.73}$$

where

$$M_{pqrs,nmkl} = \left\langle \hat{a}^{\dagger q} \hat{a}^p \hat{a}^{\dagger n} \hat{a}^m \hat{b}^{\dagger s} \hat{b}^r \hat{b}^{\dagger k} \hat{b}^l \right\rangle_{PT} = \left\langle \hat{a}^{\dagger q} \hat{a}^p \hat{a}^{\dagger n} \hat{a}^m \hat{b}^{\dagger l} \hat{b}^k \hat{b}^{\dagger r} \hat{b}^s \right\rangle. \tag{4.74}$$

Now, the criterion (4.73) takes the following matrix form

$$c \cdot M \cdot c^T \geq 0, \ \forall c \tag{4.75}$$

where $\forall c$ is equivalent to $\forall \hat{f}$ since the matrix elements of are solely dependent on $\hat{f}$. This inequality (4.75) is equivalent to saying that the matrix M is positive semi-definite, as you can see from (4.9) when we made a similar discussion regarding Simon's criterion and also described what the principal minors of a matrix are. Since M is positive semi-definite due to (4.75), we can employ Sylvester's criterion [74] and demand that *all its principal minors are non-negative*. For the definition of principal minors see the example (4.10). The matrix elements of M are defined as,

$$M_{ij} = \left\langle \hat{a}^{\dagger q} \hat{a}^{p} \hat{a}^{\dagger n} \hat{a}^{m} \hat{b}^{\dagger l} \hat{b}^{k} \hat{b}^{\dagger r} \hat{b}^{s} \right\rangle, \tag{4.76}$$

where $i = (n, m, k, l)$, $j = (p, q, r, s)$ is the ith row and jth column respectively, and we use the following numbering rule for the multi-indices,

$$i < j \;\Leftrightarrow\; \begin{cases} |i| < |j| \;\; \text{or} \\ |i| = |j| \;\; \text{and} \;\; i <' j, \end{cases} \tag{4.77}$$

where we defined $|i| = n + m + k + l$ and $i <' j$ means that the first non-zero difference $r-k, s-l, p-n, q-m$ is positive. Following these rules we find the following numeration,

	k	**l**	**n**	**m**
$i = 1$	0	0	0	0
$i = 2$	0	0	0	1
$i = 3$	0	0	1	0
$i = 4$	0	1	0	0
$i = 5$	1	0	0	0
$i = 6$	0	0	0	2
$i = 7$	0	0	1	1
$i = 8$	0	0	2	0
$i = 9$	0	1	0	1
$i = 10$	0	1	1	0
$i = 11$	0	2	0	0
$i = 12$	1	0	0	1
$i = 13$	1	0	1	0
$i = 14$	1	1	0	0
$i = 15$	2	0	0	0
$i = 16$	0	0	0	3
$i = 17$	0	0	1	2
$i = 18$	0	0	2	1
$i = 19$	0	0	3	0
$i = 20$	0	1	0	2
$i = 21$	0	1	1	1
$i = 22$	0	1	2	0
$i = 23$	0	2	0	1
	⋮			

,

	r	**s**	**p**	**q**
$j = 1$	0	0	0	0
$j = 2$	0	0	0	1
$j = 3$	0	0	1	0
$j = 4$	0	1	0	0
$j = 5$	1	0	0	0
$j = 6$	0	0	0	2
$j = 7$	0	0	1	1
$j = 8$	0	0	2	0
$j = 9$	0	1	0	1
$j = 10$	0	1	1	0
$j = 11$	0	2	0	0
$j = 12$	1	0	0	1
$j = 13$	1	0	1	0
$j = 14$	1	1	0	0
$j = 15$	2	0	0	0
$j = 16$	0	0	0	3
$j = 17$	0	0	1	2
$j = 18$	0	0	2	1
$j = 19$	0	0	3	0
$j = 20$	0	1	0	2
$j = 21$	0	1	1	1
$j = 22$	0	1	2	0
$j = 23$	0	2	0	1
		⋮		

. (4.78)

As for an example let us calculate a higher order criterion, 4th to be exact, which is already employed in [84]; if we delete the following lines and columns

$$i, j = 2, 3, 4, 6, 7, 8, 9, 10, 11, 13, \ldots \tag{4.79}$$

we get the following principal minor S which should be non-negative,

$$S = \begin{vmatrix} M_{11} & M_{15} & M_{1,12} \\ M_{51} & M_{55} & M_{5,12} \\ M_{12,1} & M_{12,5} & M_{12,12} \end{vmatrix} = \begin{vmatrix} 1 & \left\langle \hat{b}^\dagger \right\rangle & \left\langle \hat{a}\hat{b}^\dagger \right\rangle \\ \left\langle \hat{b} \right\rangle & \left\langle \hat{b}^\dagger \hat{b} \right\rangle & \left\langle \hat{a}\,\hat{b}^\dagger \hat{b} \right\rangle \\ \left\langle \hat{a}^\dagger \hat{b} \right\rangle & \left\langle \hat{a}^\dagger \hat{b}^\dagger \hat{b} \right\rangle & \left\langle \hat{a}^\dagger \hat{a}\,\hat{b}^\dagger \hat{b} \right\rangle \end{vmatrix}. \tag{4.80}$$

If we use this criterion on the following entangled quantum state, composed of two coherent states,

$$|\psi\rangle = N(\alpha,\beta)\ \left(|\alpha,\beta\rangle - |-\alpha,-\beta\rangle\right), \tag{4.81}$$

by evaluating the matrix elements in (4.80) with respect to this state, we find[84]

$$S = -|\alpha|^2|\beta|^4 \frac{\coth\left(|\alpha|^2+|\beta|^2\right)}{\sinh^2\left(|\alpha|^2+|\beta|^2\right)} \leq 0, \quad \forall \alpha,\beta \neq 0. \tag{4.82}$$

The second order criteria, of Simon and Duan *et. al.*, fail to find entanglement in this state. This specific 4th order criterion S will come in handy in *Part IV*, where we search for spatial entanglement in a thermal state of a bosonic field, as Simon's and Duan *et. al.*'s criteria will be seen to fail once more. The latter criteria are not sufficient in general when we are dealing with entanglement between number states. As a final note let us say that Simon's criterion is only a specific principal minor of the (infinite) matrix (4.76), namely

$$\begin{aligned} I_{Simon} &= \begin{vmatrix} 1 & \langle \hat{a} \rangle & \langle \hat{a}^\dagger \rangle & \left\langle \hat{b}^\dagger \right\rangle & \left\langle \hat{b} \right\rangle \\ \langle \hat{a}^\dagger \rangle & \langle \hat{a}^\dagger \hat{a} \rangle & \langle \hat{a}^{\dagger 2} \rangle & \left\langle \hat{a}^\dagger\, \hat{b}^\dagger \right\rangle & \left\langle \hat{a}^\dagger \hat{b} \right\rangle \\ \langle \hat{a} \rangle & \langle \hat{a}^2 \rangle & \langle \hat{a}\hat{a}^\dagger \rangle & \left\langle \hat{a}\,\hat{b}^\dagger \right\rangle & \left\langle \hat{a}\,\hat{b} \right\rangle \\ \left\langle \hat{b} \right\rangle & \left\langle \hat{a}\,\hat{b} \right\rangle & \left\langle \hat{a}^\dagger \hat{b} \right\rangle & \left\langle \hat{b}^\dagger \hat{b} \right\rangle & \left\langle \hat{b}^2 \right\rangle \\ \left\langle \hat{b}^\dagger \right\rangle & \left\langle \hat{a}\,\hat{b}^\dagger \right\rangle & \left\langle \hat{a}^\dagger \hat{b}^\dagger \right\rangle & \left\langle \hat{b}^{\dagger 2} \right\rangle & \left\langle \hat{b}\hat{b}^\dagger \right\rangle \end{vmatrix} \\ &= \det A\ \det B + \left(\frac{1}{4} - |\det C|\right)^2 - Tr\left[A\omega C\omega B\omega C^T J\right] - \frac{1}{4}\left(\det A + \det B\right). \end{aligned} \tag{4.83}$$

Part IV

Applications

Chapter 5

Spatial entanglement

In Part III of this Thesis we investigated various aspects of continuous variable entanglement, including various separability criteria. In this Chapter we will see these criteria in action by using them to detect continuous variable entanglement in the degrees of freedom of a quantum field. As we will discuss, there are, infinitely many, different ways to define independent degrees of freedom for a field and hence different kinds of entanglement. Since we search for spatial entanglement we need to carefully define the degrees of freedom that correspond to that kind of entanglement. This is not an easy task as seen by a major mistake we found in the literature, which we fix.

5.1 What is spatial entanglement?

In simple words, spatial entanglement means that localised regions of a system (e.g. a quantum field) exhibit particle number correlations that are non-local. This entanglement exists between the occupation number of modes and not between the particles themselves, so it's necessary to work in the second quantization formalism. Take, as an example, a photon and a beam splitter. When the photon goes through the beam splitter, its quantum state splits into two different non-overlapping regions. If we perform this experiment many times and each time measure which path the photon took, we will see that the number of times we find it in one direction and the number of times we find it in the other direction are non-locally correlated because the photon is in a superposition of both. Let's work out a simple example in order to gain a better understanding.

Example: A particle in an infinite square well

In this example we will see how we define spatial entanglement, and realize that it this kind of entanglement can exist even with just one particle making evident the fact that it's existence doesn't depend on the number of particles.

Suppose that we have one particle inside an 1D infinite square well of length L in the ground state $\varphi_0(x)$. Via Eq. (3.15) we can define the ladder operator

$$\hat{a}_0^\dagger = \int_0^L dx \varphi_0(x)\, \hat{a}_x^\dagger, \tag{5.1}$$

that creates this particle out of the vacuum $|0\rangle$

$$\hat{a}_0^\dagger |0\rangle_0 = |1\rangle_0, \tag{5.2}$$

where the symbolism $|n\rangle_0$ means that there are n particles in the ground state $\varphi_0(x)$. Now we divide the well in two regions, (L)eft and (R)ight, and for simplicity we choose to divide it in half. That way we can re-write (5.1) as

$$\hat{a}_0^\dagger = \frac{1}{\sqrt{2}} \Bigg(\underbrace{\int_0^{L/2} dx \sqrt{2} \varphi_0(x) \hat{a}_x^\dagger}_{\hat{\psi}_L^\dagger} + \underbrace{\int_{L/2}^{L} dx \sqrt{2} \varphi_0(x) \hat{a}_x^\dagger}_{\hat{\psi}_R^\dagger} \Bigg) = \frac{1}{\sqrt{2}} \left(\hat{\psi}_L^\dagger + \hat{\psi}_R^\dagger \right), \tag{5.3}$$

where we defined the independent spatial modes $\hat{\psi}_L^\dagger$, $\hat{\psi}_R^\dagger$. They are called spatial modes because they create localised particles, with $\hat{\psi}_L^\dagger$ creating a particle in region L with wavefunction $\sqrt{2}\varphi_0(x \in L)$ while $\hat{\psi}_R^\dagger$ created a particle in region R with wavefunction $\sqrt{2}\varphi_0(x \in R)$. Note that the coefficient $\sqrt{2}$ is necessary in order for the localised wavefunction to be normalised.

Now let's see what we have done from a mathematical point of view. We are working in the second quantization formalism, which means that -following the discussion at the beginning of this chapter- our space is the Fock space H_F. The operator $\hat{a}_0^\dagger$ acts on this space. When we decompose $\hat{a}_0^\dagger$ into the independent set $\{\hat{a}_x\}$, H_F breaks into an infinite tensor product

$$H = \bigotimes_{x \in [0,L]} H_x, \tag{5.4}$$

where H_x is the part of H_F that $\hat{a}_x$ acts on. The fock space H_x is spanned by the occupation number states $\{|n\rangle_x\}$ of the position eigenstate $|x\rangle$. When we further do the decomposition (5.3), H_F breaks in only two pieces

$$H_F = \bigotimes_{x \in [0,L]} H_x = \left(\bigotimes_{x \in L} H_x \right) \left(\bigotimes_{x' \in R} H_{x'} \right) = H_L \otimes H_R. \tag{5.5}$$

Correspondingly, a state that belongs two H_F breaks into a tensor product of two states, one that belongs to H_L and another that belongs to H_R, namely

$$|\,\rangle \in H_F \rightarrow |\,\rangle_L \otimes |\,\rangle_R, \tag{5.6}$$

where the notation of an empty ket denotes that the statement is true for any possible ket belonging to the corresponding Fock space. We didn't do this mathematical analysis for no reason. Now we are able to understand that the vacuum state $|0\rangle_0 \in H_F$, defined from $\hat{a}_0 |0\rangle_0 = 0$, breaks into a tensor product

$$|0\rangle_0 = |0\rangle_L \otimes |0\rangle_R, \tag{5.7}$$

where the vacuum states $|0\rangle_{L,R}$ are defined from

$$\hat{\psi}_{L(R)} |0\rangle_{L(R)} = 0, \tag{5.8}$$

meaning that there are zero particles with quantum state $\sqrt{2}\varphi_0\,(x \in L(R))$.

What we have managed to do, is to create a tensor product structure between two independent Fock spaces giving us the ability to define entanglement!

Let us act on the original vacuum $|0\rangle_0$ with $\hat{a}_0^\dagger$, creating a particle at the ground state $\varphi_0\,(x)$ of the well,

$$\begin{aligned} |1\rangle_0 = \hat{a}_0^\dagger|0\rangle_0 &= \frac{1}{\sqrt{2}}\left(\hat{\psi}_L^\dagger \otimes \hat{1}_R + \hat{1}_L \otimes \hat{\psi}_R^\dagger\right)|0\rangle_L \otimes |0\rangle_R \\ &= \frac{1}{\sqrt{2}}\left(\hat{\psi}_L^\dagger|0\rangle_L \otimes |0\rangle_R + |0\rangle_L \otimes \hat{\psi}_R^\dagger|0\rangle_R\right) \\ &= \frac{1}{\sqrt{2}}\left(|1\rangle_L \otimes |0\rangle_R + |0\rangle_L \otimes |1\rangle_R\right). \end{aligned} \tag{5.9}$$

This is an important relation if we are to understand what spatial entanglement is. We see that the ground state of the infinite square well $|1\rangle_0$ can be expressed, in the second quantization formalism, as an entangled state between two independent degrees of freedom H_L and H_R. On the one hand, H_L includes occupation number states of localised single particle state in the Left side of the well. On the other hand, H_R includes occupation number states of localised single particle states in the Right side of the well.

We have a superposition of two states:
• $|1\rangle_L \otimes |0\rangle_R = 1$ particle spatially localised in the left region L with wavefunction $\sqrt{2}\varphi_0\,(x \in L)$, and 0 particles in the right region R.
• $|0\rangle_L \otimes |1\rangle_R = 0$ particles in the left region L, and 1 particle spatially localised in the right region R with wavefunction $\sqrt{2}\varphi_0\,(x \in R)$.

If we are to use the example of the beam splitter and the photon, discussed in the beginning of this section, the Left side is the left direction that the photon may take and the Right side is the right direction.

The degrees of freedom that are entangled in (5.9) are particle numbers in different regions in space. These particle number correlations are also non-local since they can violate a Bell inequality as shown in [78]. One may object that this way of "creating" entanglement, like in (5.9), is just a mathematical trick. We will show, however, in the next chapter that this kind of entanglement, spatial entanglement, can actually be extracted from a Bose-Einstein Condensate (BEC) to a pair of independent two-level systems that could be later used for quantum information processing tasks! Besides that, spatial entanglement can be used for quantum teleportation [79] and it's also useful as a resource for quantum communication [80]. So, spatial entanglement isn't just a mathematical trick, it's there and it's useful.

Also note that, in order for spatial entanglement to exist between two regions in space there must be at least one particle whose spatial wavefunction is non zero in these two regions. For example, what would happen if we created many localised particles in the Left and Right regions of the square well alone? Would any entanglement be created? Let's see by acting on the vacuum n-times with the creation operator $\hat{\psi}_L^\dagger \otimes \hat{\psi}_R^\dagger$,

$$\left(\hat{\psi}_L^\dagger \otimes \hat{\psi}_R^\dagger\right)^n |0\rangle_L \otimes |0\rangle_R \propto |n\rangle_L \otimes |n\rangle_R. \tag{5.10}$$

No entanglement is created, hence we showed that just one delocalised particle in both the two spatial regions of interest is enough to create entanglement.

In the next section we will take the first step towards showing the usefulness of spatial entanglement and investigate whether a free non-relativistic bosonic field is spatially entangled.

5.2 Searching for spatial entanglement in a free non-relativistic bosonic field

As explained in the previous section, we want to see whether the bosonic field is spatially entangled. Since the quantum state of the field is a continuous variable state we will use the machinery of Part III, the continuous-variable entanglement criteria [82]-[84], to achieve our purpose. But first let us briefly review what a free bosonic field at finite temperature is and what it means for the field's thermal state to be spatially entangled. For a more self-contained review of the Bose-Einstein Condensate see the Appendix B.

5.2.1 The free bosonic field at finite temperature

It's well known from quantum statistical mechanics that the state of N non-interacting bosons at temperature T, in the grand-canonical ensemble formalism, is given by

$$\hat{\rho} = \exp\left[-\beta \sum_k \left(E_k - \mu\right) \hat{a}_k^\dagger \hat{a}_k\right] \Big/ Z, \tag{5.11}$$

where $\beta = 1/k_B T$, $\{\hat{a}_k\}$ are the momentum modes, $Z = Tr\hat{\rho}$ and μ is the chemical potential determined by the condition,

$$N = \sum_k \left\langle \hat{a}_k^\dagger \hat{a}_k \right\rangle = \sum_k \frac{1}{e^{\beta(E_k - \mu)} - 1}. \tag{5.12}$$

where

$$\langle \hat{n}_k \rangle = Tr\left[\hat{a}_k^\dagger \hat{a}_k \hat{\rho}\right] = \frac{1}{e^{\beta(E_k - \mu)} - 1} \tag{5.13}$$

is the mean occupation number of the single particle momentum state $|k\rangle$.

5.2.2 Spatial Entanglement

Our objective is to investigate whether the free bosonic field is spatially entangled. In order to do that we first have to understand what spatial entanglement is.

It's known[41] that entanglement is not an absolute property of a quantum state but a *relative* one, i.e. we cannot say that a state is entangled or not in general without specifying the degrees of freedom we are referring to, as we have already discussed in Section 2.6.1 when we talked about discrete-variable entanglement. In the case of continuous

variables, this is true as well. As for a most simple example, consider the hydrogen atom H_2 which is a composite system of two particles, e and p. The joint Hilbert space of H_2 is a tensor product of the Hilbert spaces of the two particles, i.e. $H = H_e \otimes H_p$. According to this tensor product structure of the single-particle degrees of freedom, these degrees of freedom are considered to be entangled in the total H_2 quantum state. However, this is not the only tensor product structure of H possible. We can make a change of coordinates from the particle degrees of freedom to the collective degrees of freedom of center of mass R and relative position r, i.e. $H = H_R \otimes H_r$. According, now, to this tensor product structure the state is considered to be separable and we conclude that entanglement is a relative property of a quantum state depending on the degrees of freedom we are referring to.

So, when we talk about spatial entanglement we are actually referring to a specific tensor product structure of the Fock space that the state belongs to. Or in other words, spatial entanglement corresponds to the entanglement of specific degrees of freedom of the bosonic field. What are these?

In the 2nd quantization formalism we introduce the ladder operators $\left\{\hat{a}_k^\dagger, \hat{a}_k\right\}$ that raise/lower the occupation number states $\{|n\rangle_k, n \in [0,\infty)\}$ of the single-particle momentum state $|k\rangle$. These ladder operators, for each k, correspond to independent degrees of freedom and they span the Fock space H. So, the Fock space breaks into an infinite tensor product structure, $H = \underset{k}{\otimes} H_k$, where $\hat{a}_k^\dagger, \hat{a}_k$ acts only on H_k. In order to define the spatial modes, rather than the momentum modes, we make a change of coordinates and define the field operators $\hat{\psi}(x)$ via

$$\hat{\psi}(x) = \int dk \, \langle x \mid k \rangle \hat{a}_k. \tag{5.14}$$

These ladder operators $\left\{\hat{\psi}^\dagger(x), \hat{\psi}(x)\right\}$ raise/lower the occupation number states $\{|n\rangle_x, n \in [0,\infty)\}$of the single particle position state $|x\rangle$ and correspond to independent degrees of freedom since they commute for different positions. The Fock space in these new coordinates has the following tensor product structure,

$$H = \underset{x\in(-\infty,+\infty)}{\otimes} H_x, \tag{5.15}$$

where $\hat{\psi}(x)$ acts only on H_x.

This structure (5.15) *defines* spatial entanglement. When we ask whether the degrees of freedom of two spatial regions, e.g. $L = (-\infty, 0]$ and $R = (0, +\infty)$ are entangled, we actually ask whether the given state $\hat{\rho}$ is entangled according to the tensor product structure

$$H = \left(\underset{x\in L}{\otimes} H_x\right)\left(\underset{x'\in R}{\otimes} H_{x'}\right). \tag{5.16}$$

In other words, if a state $\hat{\rho}$ cannot be written in the separable form

$$\hat{\rho} = \sum_i p_i \hat{\rho}_{i,L} \otimes \hat{\rho}_{i,R}, \tag{5.17}$$

where $\hat{\rho}_{i,L} \in \left(\underset{x\in L}{\otimes} H_x \right)$ and $\hat{\rho}_{i,R} \in \left(\underset{x\in R}{\otimes} H_x \right)$, then it's said to be spatially entangled. Ofcourse we can consider any two spatial regions, not just the mentioned L and R. They need not even complement the whole space, and in this case we have to take the reduced state by tracing out the modes belonging to regions other than L and R.

5.3 Short review and application of Simon's criterion

In this section we will briefly review Simon's criterion [82]. More specifically, we would like to investigate whether the thermal state (5.11) is spatially entangled with respect to the spatial modes belonging to two different regions of space, L and R, not covering all space. For example, L could be the region $L = [-10, -5]$ and $R = [5, 10]$. Following this example for clarity, the rest space r whose modes we don't consider is the region $r = (-\infty, -10) \cup (-5, 5) \cup (5, +\infty)$. By taking the reduced density matrix $\hat{\rho}_{LR} = Tr_r \hat{\rho}$ we wish to see whether $\hat{\rho}_{LR}$ can be written in the separable form (5.17).

For that purpose, we define position- and momentum-like observables $\hat{q}_i, \hat{p}_i$ $(i = L, R)$ for each region, so that $\hat{q}_i, \hat{p}_i$ act only on the Hilbert space $\left(\underset{x\in i}{\otimes} H_x \right)$ and they also satisfy

$$[\hat{q}_i, \hat{p}_j] = i\delta_{ij}. \tag{5.18}$$

We also define the 4×4 covariance matrix V of these observables,

$$V = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & C_{11} & C_{12} \\ A_{21} & A_{22} & C_{21} & C_{22} \\ C_{11} & C_{21} & B_{11} & B_{12} \\ C_{12} & C_{11} & B_{21} & B_{22} \end{pmatrix}, \tag{5.19}$$

with matrix elements given by

$$V_{ij} = \left\langle \left\{ \Delta\hat{\xi}_i, \Delta\hat{\xi}_j \right\} \right\rangle, i, j = 1, 2, 3, 4 \tag{5.20}$$

where $\hat{\xi} = \begin{pmatrix} \hat{q}_L & \hat{p}_L & \hat{q}_R & \hat{p}_R \end{pmatrix}$ and

$$\Delta\hat{\xi}_i = \hat{\xi}_i - \left\langle \hat{\xi}_i \right\rangle. \tag{5.21}$$

Simon's separability criterion corresponds to eq. (19) in [82]. It states that every separable bipartite state of the form (5.17) should satisfy the following inequality,

$$\det A \det B + \left(\frac{1}{4} - |\det C| \right)^2 - tr\left(AJCJBJC^T J \right) \geq \frac{1}{4} \left(\det A + \det B \right). \tag{5.22}$$

The 2×2 matrices A,B,C are defined in (5.19) and $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

In the case of *Gaussian states*, this criterion is proved[82] to be a necessary and sufficient condition for separability. i.e. If (5.22) is satisfied then the state is separable,

while if it's violated then it's entangled. On the other hand, in the case of *non-Gaussian states* the criterion is weaker. i.e. If (5.22) is satisfied then it gives us no information about the separability of the state, while if it's violated then the state is entangled.

Besides (5.22) which has to be satisfied by all separable states, there is[82] another inequality which is the equivalent of the uncertainty principle and has to be satisfied by *all states* regardless separability, i.e.

$$\det A \det B + \left(\frac{1}{4} - \det C\right)^2 - tr\left(AJCJBJC^T J\right) \geq \frac{1}{4}\left(\det A + \det B\right). \tag{5.23}$$

where the only difference from (5.22) is the lack of the absolute value in $\det C$. If the quantum state has $\det C > 0$ then eq. (5.22) is equivalent to (5.23) meaning that it will always be satisfied. Which means that if the state is Gaussian then it will be separable while if it's not Gaussian then we will have no information about separability.

What we have to do in the following is to calculate all the matrix elements (5.20) of the covariance matrix and see whether the inequality (5.22) is satisfied or violated. But before we do that we have to define suitable position- and momentum-like observables for each region, namely the spatial modes.Let us first see how not to define the spatial modes, taking example of a mistake in literature.

5.3.1 How Not to Define the Spatial Modes

Taking example of Peskin's[1] *How Not to Quantize the Dirac Field*, we will show how not to define the spatial modes. We mentioned in the previous section that in order to use the continuous variable criteria [82]-[84] (not only Simon's) we need to correctly define the spatial modes, i.e. operators for each subsystem that act on the specific decomposition (5.16) of the Fock space which correctly defines spatial entanglement.

L. Heaney et. al. attemped to solve this problem in [81]. They defined the following position-like operators for each region L, R

$$\hat{q}_{L(R)} = \int\limits_{L(R)} dx\, g\left(x\right) \hat{q}\left(x\right) \tag{5.24}$$

$$\hat{q}\left(x\right) = \sum_{k=1}^{\infty} \varphi_k\left(x\right) \hat{q}_k \tag{5.25}$$

$$\hat{q}_k = \sqrt{\frac{\hbar}{2m\omega_k}} \left(\hat{a}_k^\dagger + \hat{a}_k\right), \tag{5.26}$$

where $\hbar\omega_k = \hbar^2 k^2/2m$ and $\left\{\hat{a}_k, \hat{a}_k^\dagger\right\}$ are the momentum modes that lower/raise the occupation number of momentum's eigenstates $\Phi_k(x)$.

They argued that $\hat{q}\left(x\right)$ is a spatial mode for the point x in space just because this operator has the label x. It's true that $\{\hat{q}\left(x\right)\}$ is an independent set of operators for every x. However, as we have already discussed spatial entanglement has a very specific meaning and for a detailed discussion refer to the previous section. As we showed in

(3.15), for an operator to be called a spatial mode of some region L(R) it should have the form,

$$\hat{a}^{\dagger}_{L(R)} = \int\limits_{L(R)} dx g\left(x\right) \hat{a}^{\dagger}_{x}$$

or, equivalently, we could define a position-like operator for that region

$$\begin{aligned} \hat{q}'_{L(R)} &= \frac{1}{\sqrt{2}} \left(\hat{a}^{\dagger}_{L(R)} + \hat{a}_{L(R)} \right) \\ &= \frac{1}{\sqrt{2}} \left(\int\limits_{L(R)} dx g\left(x\right) \hat{a}^{\dagger}_{x} + \int\limits_{L(R)} dx g^{*}\left(x\right) \hat{a}_{x} \right). \end{aligned} \tag{5.27}$$

This means that a proper spatial mode for a region $L(R)$ should contain only those $\left\{\hat{a}_x, \hat{a}^{\dagger}_x\right\}$ for $x \in L(R)$. An analysis of (5.24) will show that this is not the case for the particular operator. If we substitute (5.26) in (5.25) and also use the Fourier decomposition $\hat{a}_k = \int dx \varphi_k\left(x\right) \hat{a}_x$ (see (3.14)) we find,

$$\hat{q}\left(x\right) = \int\limits_{-\infty}^{\infty} dx' \left(\sum_{k=1}^{\infty} \frac{\varphi_k\left(x\right) \varphi_k\left(x'\right)}{k} \right) \hat{a}^{\dagger}_{x'} + \int\limits_{-\infty}^{\infty} dx' \left(\sum_{k=1}^{\infty} \frac{\varphi_k\left(x\right) \varphi^{*}_k\left(x'\right)}{k} \right) \hat{a}_{x'}. \tag{5.28}$$

This is the important part of the argument. Since the quantity

$$\left(\sum_{k=1}^{\infty} \frac{\varphi_k\left(x\right) \varphi_k\left(x'\right)}{k} \right) \neq \delta\left(x - x'\right) \tag{5.29}$$

is not an exact delta function, due to the appearance of momentum k in the denominator, we conclude that in the observable $\hat{q}(x)$ the spatial modes $\hat{a}_x, \hat{a}^{\dagger}_x$ of **all positions**, $\forall x$, contribute and not just the x in the specific position. The situation is the same for $\hat{q}_{L(R)}$, meaning that the spatial modes $\hat{a}_x, \hat{a}^{\dagger}_x$ $\forall x$ contribute and not just those with $x \in L(R)$.

We conclude that $\hat{q}_L, \hat{q}_R$, given by (5.24), are not proper observables for the study of spatial entanglement, since they don't act on the correct decomposition of Fock space. This means that the entanglement *L. Heaney et. al.* uncover is not spatial entanglement, but entanglement between other *nonlocal* degrees of freedom. Below we set things right and define proper modes in order to apply the continuous variable criteria [82]-[84]. Unfortunately, as we will see, *Simon's* and *Duan et. al.'s* second order criteria will not be able to uncover any entanglement and we will be forced to use the higher order criteria of *Shchukin and Vogel* to detect it. We will draw conclusions from this fact about the gaussianity of the thermal state with respect to the spatial modes.

5.3.2 Defining the Spatial Modes

In order to investigate spatial entanglement with Simon's criterion (and Duan et.al.'s as well) we have to define the observables $\hat{\xi} = \begin{pmatrix} \hat{q}_L & \hat{p}_L & \hat{q}_R & \hat{p}_R \end{pmatrix}$ carefully so that the

observables $\hat{q}_L, \hat{p}_L$ act only on the part $\left(\underset{x\in L}{\otimes} H_x\right)$ of Fock space and $\hat{q}_R, \hat{p}_R$ act only on $\left(\underset{x\in R}{\otimes} H_x\right)$. We remind that the Fock space has the tensor product structure

$$H = \underbrace{\left(\underset{x\in L}{\otimes} H_x\right)}_{L-region} \underbrace{\left(\underset{x'\in R}{\otimes} H_{x'}\right)}_{R-region} \underbrace{\left(\underset{x\notin L,R}{\otimes} H_x\right)}_{rest space}. \tag{5.30}$$

Let us make a quick note at this point. Up to now we used the notation $\hat{a}_x, \hat{a}_x^\dagger$ to denote the ladder operators that lower/raise the occupation number of position's eigenstate $|x\rangle$. For a non-relativistic (Schrodinger) field it's true that the field operator $\hat{\psi}(x)$ is given by

$$\hat{\psi}(x) = \sum_k \varphi_k(x)\,\hat{a}_k, \tag{5.31}$$

and since we know from (3.14) that $\hat{a}_x = \sum_k \varphi_k(x)\,\hat{a}_k$ we conclude that

$$\begin{gathered}\hat{\psi}(x) = \hat{a}_x. \\ \text{(non-relativistically)}\end{gathered} \tag{5.32}$$

In the rest of the analysis we will use the notation $\hat{\psi}(x)$.

We will take advantage of the fact that the field operator $\hat{\psi}(x)$ at point x acts only on the part H_x of Fock space. So, an operator that acts only the part $\left(\underset{x\in i}{\otimes} H_x\right)$ of Fock space should contain only those $\hat{\psi}(x)$ for which $x \in i$. To construct such an operator we will just take a linear combination with some random weighting fuction, i.e.

$$\hat{q}_i = \frac{1}{\sqrt{2}}\left(\hat{\psi}_i + \hat{\psi}_i^\dagger\right) \tag{5.33}$$

$$\hat{p}_i = \frac{-i}{\sqrt{2}}\left(\hat{\psi}_i - \hat{\psi}_i^\dagger\right), \tag{5.34}$$

where

$$\hat{\psi}_i = \int\limits_{x\in i} dx\, g(x)\,\hat{\psi}(x) \tag{5.35}$$

with $g(x)$ being a random normalized function, $\int\limits_{x\in i} dx|g(x)|^2 = 1$. It's easy to see that the spatial modes (5.33), (5.34) we constructed satisfy the desired commutation relation $[q_i, p_j] = i\delta_{ij}$.

5.3.3 Calculation of the Covariance Matrix Elements

We remind that the thermal state of the system is

$$\hat{\rho} = \frac{1}{Z} e^{-\beta\sum\limits_k (E_k-\mu)\hat{n}_k} = \sum_{\{n_k\}} \frac{e^{-\beta\sum\limits_k (E_k-\mu)n_k}}{Z} |n_{k_1}, n_{k_2}, \ldots\rangle \langle n_{k_1}, n_{k_2}, \ldots|, \tag{5.36}$$

where we used the following decomposition of unity

$$\hat{1} = \left(\sum_{n_{k_1}} |n_{k_1}\rangle \langle n_{k_1}| \right) \otimes \left(\sum_{n_{k_2}} |n_{k_2}\rangle \langle n_{k_2}| \right) \otimes \cdots = \sum_{\{n_k\}} |n_{k_1}, n_{k_2}, \ldots\rangle \langle n_{k_1}, n_{k_2}, \ldots|. \quad (5.37)$$

Also note that $\hat{a}_k |n_k\rangle = \sqrt{n_k - 1}\, |n_k - 1\rangle$. In order to calculate the mean values of the spatial modes with respect to the state (5.36) we have to express them via the operators $\{\hat{a}_k\}$ since we know the action of the latter on$\{|n_k\rangle\}$. Using the decomposition (5.14) it's easy to see that

$$\hat{\psi}_i = \int\limits_{x \in i} dx g(x) \hat{\psi}(x) = \sum_k \int\limits_{x \in i} dx g(x) \langle x \mid k \rangle \hat{a}_k. \quad (5.38)$$

It's easy to see that

$$\langle \hat{q}_i \rangle = \langle \hat{p}_i \rangle = 0 \quad (5.39)$$

since only matrix elements of the form $\langle n_{k_1}, n_{k_2}, \ldots| \hat{a}_k^{(\dagger)} |n_{k_1}, n_{k_2}, \ldots\rangle$ are contained, so that $\Delta\hat{\xi}_i = \hat{\xi}_i - \left\langle \hat{\xi}_i \right\rangle = \hat{\xi}_i$ and

$$V_{ij} = \frac{1}{2} \left(\hat{\xi}_i \hat{\xi}_j + \hat{\xi}_j \hat{\xi}_i \right). \quad (5.40)$$

The matrix elements are:

$$\bullet V_{ii} = \left\langle \hat{\xi}_i^2 \right\rangle, \quad i = 1, 2, 3, 4 \quad (5.41)$$

$$\bullet V_{12} = V_{21} = \frac{1}{2} \langle \hat{q}_L \hat{p}_L + \hat{p}_L \hat{q}_L \rangle = 0 \quad (5.42)$$

$$\bullet V_{34} = V_{43} = \frac{1}{2} \langle \hat{q}_R \hat{p}_R + \hat{p}_R \hat{q}_R \rangle = 0 \quad (5.43)$$

$$\bullet V_{13} = V_{31} = \langle \hat{q}_L \hat{q}_R \rangle = \langle \hat{p}_L \hat{p}_R \rangle = V_{24} = V_{42} = \frac{1}{2} \left(\left\langle \hat{\psi}_L \hat{\psi}_R^\dagger \right\rangle + \left\langle \hat{\psi}_L^\dagger \hat{\psi}_R \right\rangle \right) \quad (5.44)$$

$$\bullet V_{14} = V_{41} = -V_{32} = -V_{23} = \langle \hat{q}_L \hat{p}_R \rangle = \frac{i}{2} \left(\left\langle \hat{\psi}_L \hat{\psi}_R^\dagger \right\rangle - \left\langle \hat{\psi}_L^\dagger \hat{\psi}_R \right\rangle \right) \quad (5.45)$$

$$(5.46)$$

It holds that,

$$\left\langle \hat{\psi}_L \hat{\psi}_R^\dagger \right\rangle = \sum_k I_k^{R*} I_k^L \langle \hat{n}_k \rangle, \quad \left\langle \hat{\psi}_L^\dagger \hat{\psi}_R \right\rangle = \sum_k I_k^{L*} I_k^R \langle \hat{n}_k \rangle \quad (5.47)$$

where

$$I_k^i = \int\limits_{x \in i} dx g(x) \langle x \mid k \rangle. \quad (5.48)$$

The diagonal elements are

$$\left\langle \hat{q}_i^2 \right\rangle = \left\langle \hat{p}_i^2 \right\rangle = \frac{1}{2} \left\langle \hat{\psi}_i^2 + \hat{\psi}_i^{\dagger 2} \right\rangle + \left\langle \hat{\psi}_i^\dagger \hat{\psi}_i \right\rangle + \frac{1}{2} = \sum_{\{n_k\}} \langle n_{k_1}, n_{k_2}, \ldots | \hat{\rho} \hat{\psi}_i^\dagger \hat{\psi}_i | n_{k_1}, n_{k_2}, \ldots \rangle + \frac{1}{2}$$

$$= \frac{1}{2} + \sum_k \left|I_k^i\right|^2 \underbrace{\left(\sum_{\{n_k\}} n_k \frac{e^{-\beta(E_k-\mu)n_k}}{Z} \right)}_{\langle \hat{n}_k \rangle} = \frac{1}{2} + \sum_k \left|I_k^i\right|^2 \langle \hat{n}_k \rangle$$

$$= \frac{1}{2} + \sum_k \left|I_k^i\right|^2 \frac{1}{e^{\beta(E_k-\mu)} - 1}. \tag{5.49}$$

Calculation of $\det C$ gives

$$\det C = V_{13} \cdot V_{24} - V_{14} \cdot V_{23} = (V_{13})^2 + (V_{14})^2 \geq 0, \tag{5.50}$$

where we used equations (5.44),(5.45). Since $\det C \geq 0$ the separability criterion (5.22) is equivalent to the uncertainty principle (5.23) meaning that the former will always be satisfied for every value of its parameters, i.e. every temperature, separation distance of the regions, etc. Notice that the determinant is non-negative regardless of the state with respect to which the mean values are taken. So, even we assume that bosonic field is described, not by the grand-canonical ensemble as above but, by a pure state where all the bosons occupy the ground state, i.e. $|N, 0, 0, \ldots\rangle$ (absolute zero), the criterion will not be violated.

Since it has been proved in [86]-[89] that for every temperature $T \geq 0$ the field's thermal state is spatially entangled we conclude that the thermal state *must be non-Gaussian* with respect to the defined spatial modes (5.33), (5.34) and the separability criterion cannot tell us anything about the separability of the state. As we will see in the next section, this is also the case for *Duan et. al.'s* criterion concluding that the second order criteria are unable to uncover the entanglement of this non-Gaussian state. Then we will use a 4^{rth} order criterion of [84] which actually detects entanglement near the absolute zero $T = 0\ K$, proving indirectly the non-Gaussianity of the thermal state with respect to the spatial modes.

5.4 Applying *Duan et. al.'s* criterion

Now let's apply Duan et. al.'s second-order criterion[83]. For a quick review see *Part III* of the Thesis. We remind the reader that, according to this criterion, entanglement exists if the following inequality is violated

$$\left\langle (\Delta \hat{u})^2 \right\rangle_{\hat{\rho}} + \left\langle (\Delta \hat{v})^2 \right\rangle_{\hat{\rho}} \geq a^2 + \frac{1}{a^2}, \quad \text{for any} \ \ a \in R, \tag{5.51}$$

where

$$\hat{u} = |a|\, \hat{q}_L + \frac{1}{a} \hat{q}_R, \quad \hat{v} = |a|\, \hat{p}_L - \frac{1}{a} \hat{p}_R. \tag{5.52}$$

The position- and momentum-like operators are given by (5.33) and (5.34) respectively, and we'll use exactly the same notation as in Simon's criterion. Next we define the quantity

$$I_{Duan} = \left\langle (\Delta \hat{u})^2 \right\rangle_{\hat{\rho}} + \left\langle (\Delta \hat{v})^2 \right\rangle_{\hat{\rho}} - a^2 - \frac{1}{a^2}, \tag{5.53}$$

and we want to see whether it's positive or negative. We substitute the $\hat{u}, \hat{v}$ operators and get

$$I_{Duan} = a^2 \left(\langle \hat{q}_L^2 \rangle + \langle \hat{p}_L^2 \rangle - 1 \right) + \frac{1}{a^2} \left(\langle \hat{q}_R^2 \rangle + \langle \hat{p}_R^2 \rangle - 1 \right) + \\ + 2\frac{|a|}{a} \left(\langle \hat{q}_L \hat{q}_R \rangle - \langle \hat{p}_L \hat{p}_R \rangle \right). \quad (5.54)$$

Using the fact that $\left\langle \hat{\psi}_i^\dagger \hat{\psi}_i \right\rangle = \sum_k |I_k^i|^2 \langle \hat{n}_k \rangle \geq 0$ (see Eq.(5.47)) we conclude from (5.49) that

$$\langle \hat{q}_i^2 \rangle = \langle \hat{p}_i^2 \rangle = \frac{1}{2} + \left\langle \hat{\psi}_i^\dagger \hat{\psi}_i \right\rangle \geq \frac{1}{2}. \quad (5.55)$$

What this means is that the first two terms in I_{Duan} are non-negative for every a. The third, and last, term is zero due to (5.44) so we arrive at the conclusion that the criterion is never violated, i.e.

$$I_{Duan} \geq 0, \quad \forall a, \quad (5.56)$$

meaning that it cannot detect any spatial entanglement. This result holds for every state where the mean value, $\left\langle \hat{\psi}(x) \right\rangle$, of the field operator is zero. So, it holds for the grand-canonical ensemble for every value of its parameters (i.e. temperature, separation distance of the two regions e.t.c.), and it also holds for a pure state where all the bosons occupy the ground state (i.e. at absolute zero $T = 0\ K$) described by the canonical ensemble where the total number of particles is not fluctuating.

5.5 Cannot we just prove that it's non-Gaussian?

In the previous sections we saw that neither Simon's nor Duan *et. al.*'s criteria can be violated. Remember that if the quantum state in question is Gaussian then this non-violation implies separability and absence of entanglement, while if it's non-Gaussian then the non-violation implies ignorance, i.e. the criteria cannot tell us anything about the existence of entanglement. However we worked indirectly and concluded that the state *has* to be non-Gaussian because in the literature -using other methods- entanglement was detected for $T \geq 0\ K$. We took the existence of entanglement as granted, and concluded that the non-violation of the 2^{nd}-order criteria imply, not separability, but that the state is non-Gaussian. The following question comes naturally; why don't we just prove whether the quantum state (5.36) is (non-)Gaussian?

Let us first clear up some misconceptions about the Gaussianity of a quantum state. It can be shown that the thermal state

$$\hat{\rho} = \frac{1}{Z} \exp\left[-\beta\omega \left(\hat{a}^\dagger \hat{a} - \frac{1}{2} \right) \right], \quad (5.57)$$

is Gaussian. So, does this mean that this state is not spatially entangled, for any temperature, since it cannot violate the above criteria? No, this conclusion is wrong because the gaussianity was proved with respect to the energy modes $\{\hat{a}\}$ that are present in (5.57), NOT the spatial modes $\left\{ \hat{\psi}_i \right\}$. Put it simply; whether a quantum state is

Gaussian depends on the coordinates we are working with. For example, a wavefunction that is Gaussian in position space (i.e. $\psi(x)$: Gaussian function of x), may not be Gaussian with respect to some other basis, like the Hamiltonian's eigenstates (i.e. $\psi(E) = \int dx\, \varphi_E^*(x)\, \psi(x)$: may not be a Gaussian function of E). In fact, Gaussianity is preserved if the transformation from one basis to another is a Fourier transformation. So, the Gaussianity of the state is not an absolute property of the state but a relative one, in the sense that it depends entirely on the coordinate system (choice of basis).

Having that said, we can now understand that whether the thermal state is Gaussian with respect to the energy modes (in the basis defined by the eigenstates of the operator $\hat{q}_a = \frac{1}{\sqrt{2}}\left(\hat{a} + \hat{a}^\dagger\right)$) is irrelevant to whether it's Gaussian to the spatial modes (in the basis defined by the eigenstates of the operator (5.33)), since these two modes are not connected via a Fourier transform that preserves Gaussianity. The important thing is that the criteria of Simon and Duan *et. al.* require the Gaussianity of the state in the basis defined by the modes used in the criterion, i.e. the Wigner function,

$$W(\xi) \sim \exp\left(-\frac{1}{2}\xi^T V^{-1}\xi\right), \tag{5.58}$$

to be a Gaussian function of $\xi = \begin{pmatrix} q_1 & p_1 & q_2 & p_2 \end{pmatrix}$, where the q_i, p_i are the modes chosen in the criterion and V the covariance matrix of these modes. In our case, we are searching for spatial entanglement and are using the spatial modes (5.33), (5.34), so we have to prove the Gaussianity of the thermal state (5.58) with respect to these modes. However this calculation is difficult, and that's most easily seen in another formalism of the characteristic function. The exact calculation that needs to be done is to show that the characteristic function $\chi_\rho(\xi)$ of the thermal state (5.36), namely

$$\chi_\rho(\xi) = Tr\left[\hat{\rho}\; e^{i\xi_1\hat{p}_L - i\xi_2\hat{q}_L + i\xi_3\hat{p}_R - i\xi_4\hat{q}_R}\right] \tag{5.59}$$

is a Gaussian function of ξ_i. The main difficulty lies to the fact that the Hamiltonian on the exponential of the thermal state cannot be expressed solely via the spatial modes, making the actual calculation quite non-trivial.

5.6 Use of 4^{th}-order criteria to detect spatial entanglement

Up to now, correlations of moments up to the second-order were not able to reveal spatial entanglement for any temperature. In this section we will use the stronger criteria of *Shchukin* and *Vogel* [84] that we introduced in *Part III*. In particular we will use the subdeterminant S (4.80) that includes moments up to 4^{th}-order,

$$S = \begin{vmatrix} 1 & \left\langle \hat{b}^\dagger \right\rangle & \left\langle \hat{a}\hat{b}^\dagger \right\rangle \\ \left\langle \hat{b} \right\rangle & \left\langle \hat{b}^\dagger\hat{b} \right\rangle & \left\langle \hat{a}\hat{b}^\dagger\hat{b} \right\rangle \\ \left\langle \hat{a}^\dagger\hat{b} \right\rangle & \left\langle \hat{a}^\dagger\hat{b}^\dagger\hat{b} \right\rangle & \left\langle \hat{a}^\dagger\hat{a}\,\hat{b}^\dagger\hat{b} \right\rangle \end{vmatrix}, \tag{5.60}$$

where $\hat{a}$, $\hat{b}$ are the annihilation operators of the first and the second mode respectively. Since we are looking for spatial entanglement we will use the spatial modes (5.35),

$$\hat{a} = \hat{\psi}_L = \int\limits_L dx\, g\left(x\right) \hat{\psi}\left(x\right) \tag{5.61}$$

$$\hat{b} = \hat{\psi}_R = \int\limits_R dx\, g\left(x\right) \hat{\psi}\left(x\right). \tag{5.62}$$

For simplicity we will work in one spatial dimension but the results are easily generalized in three dimensions. The subdeterminant now reads

$$\begin{aligned} S &= \begin{vmatrix} 1 & 0 & \left\langle \hat{\psi}_L \hat{\psi}_R^\dagger \right\rangle \\ 0 & \left\langle \hat{\psi}_R^\dagger \hat{\psi}_R \right\rangle & 0 \\ \left\langle \hat{\psi}_L^\dagger \hat{\psi}_R \right\rangle & 0 & \left\langle \hat{\psi}_L^\dagger \hat{\psi}_L\, \hat{\psi}_R^\dagger \hat{\psi}_R \right\rangle \end{vmatrix} \\ &= \left\langle \hat{\psi}_R^\dagger \hat{\psi}_R \right\rangle \left(\left\langle \hat{\psi}_L^\dagger \hat{\psi}_L\, \hat{\psi}_R^\dagger \hat{\psi}_R \right\rangle - \left\langle \hat{\psi}_L^\dagger \hat{\psi}_R \right\rangle \left\langle \hat{\psi}_L \hat{\psi}_R^\dagger \right\rangle \right), \end{aligned} \tag{5.63}$$

and the negativity of this expression, $S < 0$ will unveil any existing entanglement. Using the decomposition of the field operator, $\hat{\psi}\left(x\right) = \sum\limits_k \varphi_k\left(x\right) \hat{a}_k$, and the notation $I_k^i = \int\limits_L dx\, g\left(x\right) \varphi_k\left(x\right)$, $\hat{N}_k \equiv \hat{a}_k^\dagger \hat{a}_k$ we find

$$\begin{aligned} \left\langle \hat{\psi}_L^\dagger \hat{\psi}_L\, \hat{\psi}_R^\dagger \hat{\psi}_R \right\rangle = \sum_{k \neq k'} I_k^L I_k^R I_{k'}^L I_{k'}^R \left(\left\langle \hat{N}_k \right\rangle \left\langle \hat{N}_{k'} \right\rangle + \left\langle \hat{N}_k \right\rangle \right) + \\ + \sum_{k \neq k'} \left(I_k^L\right)^2 \left(I_{k'}^R\right)^2 \left\langle \hat{N}_k \right\rangle \left\langle \hat{N}_{k'} \right\rangle + \sum_k \left(I_k^L\right)^2 \left(I_k^R\right)^2 \left\langle \hat{N}_k^2 \right\rangle, \end{aligned} \tag{5.64}$$

$$\left\langle \hat{\psi}_L\, \hat{\psi}_R^\dagger \right\rangle = \sum_k I_k^L I_k^R \left(1 + \left\langle \hat{N}_k \right\rangle \right), \quad \text{and} \tag{5.65}$$

$$\left\langle \hat{\psi}_L^\dagger \hat{\psi}_R \right\rangle = \sum_k I_k^L I_k^R \left\langle \hat{N}_k \right\rangle. \tag{5.66}$$

For a detailed analysis of the algebra involved see the end of Section 6.5.1. Substituting back in (5.63) we get the following expression.

$$\begin{aligned} S = &- \left(\sum_a \left(I_a^R\right)^2 \left\langle \hat{N}_a \right\rangle \right) \times \\ &\times \left[\sum_k \left(I_k^L\right)^2 \left(I_k^R\right)^2 \left[\left\langle \hat{N}_k \right\rangle - \left(\left\langle \hat{N}_k^2 \right\rangle - \left\langle \hat{N}_k \right\rangle^2 \right) \right] - \sum_{k \neq k'} \left(I_k^L\right)^2 \left(I_{k'}^R\right)^2 \left\langle \hat{N}_k \right\rangle \left\langle \hat{N}_{k'} \right\rangle \right] \end{aligned} \tag{5.67}$$

This formula surely can be negative but we will leave the analysis for Chapter 6, where we will talk about entanglement extraction out of Bose-Einstein Condensate (BEC) using

a pair of mutually independent 2-level quantum probes. It will, surprisingly, turn out that the existense of the induced entanglement between the two probes -given by (6.116)- behaves exactly the same way as the subdeterminant S!

In other words, when S is negative, meaning that the field is spatially entangled, then the two quantum probes get entangled as well. Moreover, the more negative S be the more entangled the probes get! On the other hand, if S is positive, meaning that we can't know whether there is spatial entanglement, the two quantum probes cannot get entangled. This equivalence is surprising and strongly motivates for further research. For the rest of the analysis on the existence of entanglement see Section 6.5.3; all the conclusions of that section about the existense of entanglement between the two probes apply directly to the field's spatial entanglement, since *negativity* (6.116) (which we will introduce later on) and the subdeterminant S behave identically.

Chapter 6

Entanglement extraction out of a BEC

In this chapter, we will investigate whether a non-interacting bosonic field is spatially entangled in an indirect way. We will use two independent quantum probes (which are 2-level systems) and send them to, simultaneously, interact locally with the field via an experimentally realizable interaction Hamiltonian. After the interaction we will search for entanglement in the reduced state of the probes and see how it dependents on the field's temperature and the probes' separation distance. Whatever entanglement we find must have come from the bosonic field, which will mean that the field is spatially entangled. A surprising link is found between the 4^{th}-order continuous variable entanglement criteria, we used for the field in Chapter 5, and the entanglement of the probes. Finally, we will look for a connection between the amount of the extracted entanglement and the quantum phase transition of the bosonic field.

6.1 Introduction

Entanglement is a crucial property in the field of Quantum Information, if we are to take full advantage of quantum effects. Whether you want to run fast quantum algorithms in a quantum computer, or to safely communicate via quantum cryptography or, just, test Bell's inequalities you will need to have entangled pairs of qubits. This motivates us to try and look for ways to entangle quantum systems.

An idea explored in the literature is to take advantage of a system which already has entangled degrees of freedom, and let our quantum systems interact with those degrees of freedom in a way that will make them entangled. These schemes are called *entanglement extraction* schemes, since the entanglement between between the qubits was actually extracted from the system. In this context the quantum systems, that represent our qubits, are called *quantum probes*. Various such studies appear in the literature; In [90] Reznik considered a pair of causally disconnected probes that locally interact with the vacuum of a spinless relativistic field. He showed that even when the probes are initially non-entangled, they can wind up to a final entangled state after the interaction showing that entanglement persists even between causally disconnected regions in the vacuum. In [91] Kaszlikowski *et. al.* considered local entanglement extraction from a system in a coherent state, showing that "classical" coherent states aren't so classical after all,

while in [92], [93] entanglement extraction from an ion chain and a solid was studied respectively.

In this project our main motivation in entangling probes through the process of entanglement extraction by another system -besides their usefulness in Quantum Information- will be the study of that system's entanglement properties. In particular, the system under study will be a spinless non-relativistic bosonic field at finite temperature. In the previous chapter, we studied the spatial entanglement properties of this quantum field via continuous variable entanglement criteria applied directly on the field. Only criteria of 4^{th}-order gave us a hint of entanglement existence (see Sec. 5.6). In this chapter, we will study the field's spatial entanglement properties indirectly by using the process of entanglement extraction.

Consider our probes to be a pair of initially independent, two-level and distinguishable quantum systems that are localized in space. We will let them to *locally* interact with the bosonic field for a small amount of time , but never with each other. The field is considered to be in a thermal state at temperature T. After the interaction, we study the quantum state of the probes and look for correlations. Classically, in the case where the two probes were in causally connected regions, we wouldn't be surprised if we found some correlations between the probes, but these correlations would be classical in nature. In the present consideration we will find something more. We will prove that the two probes are indeed correlated but more powerfully than classically possible, i.e. they are *entangled*. This quantum property appears even though the probes never directly directly, and also it is independent of whether the localized probes are separated by a space-like or time-like distance. Thus we show that entanglement exists between causally disconnected regions of the field's thermal state.

6.2 The model Hamiltonian

We consider our quantum probes to be two distinguishable 2-level systems with two possible internal states $\{|0\rangle, |1\rangle\}$ each, and also define the ladder operators

$$\begin{array}{l} \hat{b}^{\dagger}|0\rangle = |1\rangle, \hat{b}|1\rangle = |0\rangle \ \left(\left[\hat{b}, \hat{b}^{\dagger}\right] = 1\right) \\ \hat{c}^{\dagger}|0\rangle = |1\rangle, \hat{c}|1\rangle = |0\rangle \ \left(\left[\hat{c}, \hat{c}^{\dagger}\right] = 1\right) \end{array} \tag{6.1}$$

for the first and second probe respectively. The operators $\hat{b}$ and $\hat{c}$ that satisfy (6.1) have the form

$$\hat{b} = |0\rangle_{bb}\langle 1|, \quad \hat{c} = |0\rangle_{cc}\langle 1|, \tag{6.2}$$

which means that

$$\hat{b}^2 = \hat{c}^2 = \hat{b}^{\dagger 2} = \hat{c}^{\dagger 2} = 0. \tag{6.3}$$

Moreover, assume that the localized and non-overlapping wavefunctions of the two probes in the position basis are $\psi_b(\vec{x})$ and $\psi_c(\vec{x})$ respectively, while the free Hamiltonian of the probes is H_{probes}.

Next consider a non-relativistic free bosonic field $\hat{\Psi}_a(\vec{x})$ at finite temperature T being in the thermal state

$$\hat{\rho}_{th} = \exp\left(-\beta \hat{H}_{th}\right) \Big/ Z = \exp\left[-\beta \sum_k \left(E_k - \mu\right) \hat{a}_k^\dagger \hat{a}_k\right] \Big/ Z, \tag{6.4}$$

where $\beta = 1/k_B T$, $\{\hat{a}_k\}$ are the energy modes, $Z = Tr\hat{\rho}$ and μ is the chemical potential determined by the condition,

$$N = \sum_k \left\langle \hat{a}_k^\dagger \hat{a}_k \right\rangle = \sum_k \frac{1}{e^{\beta(E_k - \mu)} - 1} \tag{6.5}$$

where

$$\langle \hat{n}_k \rangle = Tr\left[\hat{\rho}_{th} \hat{a}_k^\dagger \hat{a}_k\right] = \frac{1}{e^{\beta(E_k - \mu)} - 1} \tag{6.6}$$

is the mean occupation number of the singe particle energy eigenstate $|k\rangle$.

Now that we have defined our systems we assume the following local interaction Hamiltonian between the bosonic field and the quantum probes,

$$H_I = H_I^{(b)} + H_I^{(c)} \tag{6.7}$$

where

$$H_I^{(b)} = \int_b d^3x \left(\hat{\Psi}_a\left(\vec{x}\right) \psi_b\left(\vec{x}\right) \hat{b}^\dagger + \hat{\Psi}_a^\dagger\left(\vec{x}\right) \psi_b\left(\vec{x}\right) \hat{b}\right) \tag{6.8}$$

$$H_I^{(c)} = \int_c d^3x \left(\hat{\Psi}_a\left(\vec{x}\right) \psi_c\left(\vec{x}\right) \hat{c}^\dagger + \hat{\Psi}_a^\dagger\left(\vec{x}\right) \psi_c\left(\vec{x}\right) \hat{c}\right). \tag{6.9}$$

Notice that the interaction Hamiltonian between the bosonic field and the probe i is integrated in the volume i where the probe's localized wavefunction $\psi_i\left(\vec{x}\right)$ is non-zero. Also note that the probes' wavefunctions are non-overlapping so it holds that $\left[H_I^{(b)}, H_I^{(c)}\right] = 0$. What this means is that the two probes interact with independent degrees of freedom and not with each other. How this Hamiltonian can be realized in an experimental setting will be discussed in a later section.

For future convenience and without losing generality, we will assume that each $\psi_i\left(\vec{x}\right)$ is constant in the volume V_i where it's non-zero. So we have,

$$\psi_i\left(\vec{x}\right) = \frac{1}{\sqrt{V_i}} \tag{6.10}$$

so that $\int\limits_i \left|\psi_i\left(\vec{x}\right)\right|^2 d^3x = 1$

We will assume that, initially, the quantum probes both are in the ground state, i.e. $|00\rangle \equiv |0\rangle_b \otimes |0\rangle_c$ and not correlated, while the bosonic field is in the thermal state $\hat{\rho}_{th}$ so that the quantum state of the whole system at time $t = 0$ can be written as

$$\hat{\rho}\left(0\right) = \hat{\rho}_{th} \otimes |00\rangle_{bcbc} \langle 00| . \tag{6.11}$$

Next we consider an interaction of short duration δt between the probes and the bosonic field, where the interaction Hamiltonian (6.7) is switched on at $t_i = 0$ and switched off at $t_f = \delta t$. This process is described by the time-dependent total Hamiltonian

$$H(t) = H_{free} + \Gamma(t) H_I \tag{6.12}$$

where $H_{free} = H_{th} + H_{probes}$ is the free Hamiltonian of the bosonic field and the probes, and $\Gamma(t)$ is non-zero only in the time interval $(0, \delta t)$. The evolution operator will be,

$$\hat{U}(\delta t) = \exp\left[-i \int_0^{\delta t} dt \left(\hat{H}_{free} + \Gamma(t) \hat{H}_I\right)\right] = \exp\left[-i\hat{H}_{free}\delta t - i\Gamma\hat{H}_I\right] \tag{6.13}$$

where $\Gamma = \int_0^{\delta t} \Gamma(t)\, dt$. We will assume that the function $\Gamma(t)$ is sharp enough in the time interval $(0, \delta t)$ so that we will be able to make the approximation $H(t) = H_{free} + \Gamma(t) H_I \approx \Gamma(t) H_I$, and consequently

$$\hat{U}(\delta t) = \exp\left[-i\hat{H}_{free}\delta t - i\Gamma\hat{H}_I\right] \approx \exp\left[-i\Gamma\hat{H}_I\right]. \tag{6.14}$$

What this means is that in the short interaction interval δt the free evolution of both the bosonic field and the probes is negligible compared to its interaction energy with the two quantum probes. Moreover, we also assume that while $\Gamma(t)$ is sharp enough to make the field's free evolution negligible it's also small enough so that the following limits hold,

$$\delta t \ll 1, \quad \Gamma = \int_0^{\delta t} \Gamma(t)\, dt \ll 1. \tag{6.15}$$

In the limit $\Gamma \ll 1$ we can taylor expand the evolution operator (6.14) and keep terms up to second order $\mathrm{O}(\Gamma^2)$,

$$\hat{U}(\delta t) = \exp\left[-i\Gamma\hat{H}_I\right] = 1 - i\Gamma\hat{H}_I - \frac{\Gamma^2}{2}\hat{H}_I^2 + \mathrm{O}\left(\Gamma^3\right). \tag{6.16}$$

It's easy to see that the unitarity of this operator is conserved up to the second order,

$$\hat{U}^\dagger(\delta t)\,\hat{U}(\delta t) = 1 + \mathrm{O}\left(\Gamma^3\right). \tag{6.17}$$

The time-evolved density matrix of the total system will be,

$$\begin{aligned}
\hat{\rho}(\delta t) &= \hat{U}(\delta t)\,\hat{\rho}(0)\,\hat{U}^\dagger(\delta t) = \\
&= \left(1 - i\Gamma\hat{H}_I - \frac{\Gamma^2}{2}\hat{H}_I^2 + \mathrm{O}\left(\Gamma^3\right)\right)\hat{\rho}(0)\left(1 + i\Gamma\hat{H}_I - \frac{\Gamma^2}{2}\hat{H}_I^2 + \mathrm{O}\left(\Gamma^3\right)\right) \\
&\approx \hat{\rho}(0) - i\Gamma\left(\hat{H}_I\hat{\rho}(0) - \hat{\rho}(0)\,\hat{H}_I\right) - \frac{\Gamma^2}{2}\hat{H}_I^2\hat{\rho}(0) - \frac{\Gamma^2}{2}\hat{\rho}(0)\,\hat{H}_I^2 + \Gamma^2\hat{H}_I\hat{\rho}(0)\,\hat{H}_I,
\end{aligned} \tag{6.18}$$

where in the last equation we have considered the terms of order $\mathrm{O}(\Gamma^3)$ to be negligible and $\hat{\rho}(0)$ is given by (6.11).

Since we are interested in the existence of the entanglement between the two probes, we trace out the bosonic field's degrees of freedom in order to get the reduced density matrix $\hat{\rho}_{bc}(\delta t)$ after the interaction. So, we get

$$\begin{aligned}\hat{\rho}_{bc}(\delta t) &= Tr_a\left[\hat{\rho}(\delta t)\right] \\ &= Tr_a\left[\hat{\rho}(0)\right] - i\Gamma Tr_a\left[\hat{H}_I\hat{\rho}(0) - \hat{\rho}(0)\hat{H}_I\right] - \frac{\Gamma^2}{2}Tr_a\left[\hat{H}_I^2\hat{\rho}(0)\right] - \\ &\quad - \frac{\Gamma^2}{2}Tr_a\left[\hat{\rho}(0)\hat{H}_I^2\right] + \Gamma^2 Tr_a\left[\hat{H}_I\hat{\rho}(0)\hat{H}_I\right]. \end{aligned} \tag{6.19}$$

Our first goal is to compute Eq.(6.19), and that we will do by considering each term separately. We define the following quantities,

$$\begin{aligned} &A_1 = Tr_a\left[\hat{\rho}(0)\right], \quad A_2 = Tr_a\left[\hat{H}_I\hat{\rho}(0) - \hat{\rho}(0)\hat{H}_I\right], \\ &A_3 = Tr_a\left[\hat{\rho}(0)\hat{H}_I^2\right], \quad A_4 = Tr_a\left[\hat{H}_I^2\hat{\rho}(0)\right], \quad A_5 = Tr_a\left[\hat{H}_I\hat{\rho}(0)\hat{H}_I\right]. \end{aligned} \tag{6.20}$$

Calculation of A_1

$$\begin{aligned} A_1 &= Tr_a\left[\hat{\rho}(0)\right] = (Tr_a\hat{\rho}_{th})\cdot|00\rangle\langle 00| \\ &= |00\rangle\langle 00| \end{aligned} \tag{6.21}$$

since $Tr_a\hat{\rho}_{th} = 1$.

Calculation of A_2

$$\begin{aligned} A_2 &= Tr_a\left[\hat{H}_I\hat{\rho}(0) - \hat{\rho}(0)\hat{H}_I\right] \\ &= \frac{1}{\sqrt{V_b}}\int_b d^3x Tr_a\left[\hat{\Psi}_a(\vec{x})\hat{\rho}_{th}\right]\hat{b}^\dagger|00\rangle\langle 00| + \frac{1}{\sqrt{V_b}}\int_b d^3x Tr_a\left[\hat{\Psi}_a^\dagger(\vec{x})\hat{\rho}_{th}\right]\hat{b}|00\rangle\langle 00| + \\ &\quad + \frac{1}{\sqrt{V_c}}\int_c d^3x Tr_a\left[\hat{\Psi}_a(\vec{x})\hat{\rho}_{th}\right]\hat{c}^\dagger|00\rangle\langle 00| + \frac{1}{\sqrt{V_c}}\int_c d^3x Tr_a\left[\hat{\Psi}_a^\dagger(\vec{x})\hat{\rho}_{th}\right]\hat{c}|00\rangle\langle 00| - \\ &\quad - \frac{1}{\sqrt{V_b}}\int_b d^3x Tr_a\left[\hat{\rho}_{th}\hat{\Psi}_a(\vec{x})\right]|00\rangle\langle 00|\hat{b}^\dagger - \frac{1}{\sqrt{V_b}}\int_b d^3x Tr_a\left[\hat{\rho}_{th}\hat{\Psi}_a^\dagger(\vec{x})\right]|00\rangle\langle 00|\hat{b} - \\ &\quad - \frac{1}{\sqrt{V_c}}\int_c d^3x Tr_a\left[\hat{\rho}_{th}\hat{\Psi}_a(\vec{x})\right]|00\rangle\langle 00|\hat{c}^\dagger - \frac{1}{\sqrt{V_c}}\int_c d^3x Tr_a\left[\hat{\rho}_{th}\hat{\Psi}_a^\dagger(\vec{x})\right]|00\rangle\langle 00|\hat{c} \\ &= 0 \quad \Leftrightarrow \end{aligned}$$

$$A_2 = 0. \tag{6.22}$$

The total result is zero, and more precisely each term separately is zero, because the mean value of the field operator with respect to the thermal state is zero. Let's prove this fact. We will use the field operator's decomposition to energy modes,

$$\hat{\Psi}_a(\vec{x}) = \sum_k \varphi_k(\vec{x})\,\hat{a}_k. \tag{6.23}$$

Since the thermal state can be decomposed as

$$\hat{\rho}_{th} = \frac{1}{Z}e^{-\beta\hat{H}_{free}} = \sum_{\{n_i\}} \frac{e^{-\beta E_{\{n_i\}}}}{Z} |n_1, n_2, \ldots\rangle \langle n_1, n_2, \ldots|, \tag{6.24}$$

we get

$$\begin{aligned} \left\langle \hat{\Psi}_a(\vec{x}) \right\rangle_{th} &= Tr_a\left[\hat{\rho}_{th}\hat{\Psi}_a(\vec{x})\right] = \sum_k \varphi_k(\vec{x}) Tr_a\left[\hat{\rho}_{th}\hat{a}_k\right] \\ &= \sum_k \varphi_k(\vec{x}) \sum_{\{n_i\}} \frac{e^{-\beta E_{\{n_i\}}}}{Z} \langle n_1, n_2, \ldots| \hat{a}_k |n_1, n_2, \ldots\rangle = 0, \end{aligned} \tag{6.25}$$

since $\langle n_1, n_2, \ldots| \hat{a}_k |n_1, n_2, \ldots\rangle = 0$. In the same way we can show

$$\left\langle \hat{\Psi}_a^\dagger(\vec{x}) \right\rangle_{th} = \left\langle \hat{\Psi}_a(\vec{x}) \right\rangle_{th} = 0. \tag{6.26}$$

Calculation of A_3

$$A_3 = Tr_a\left[\hat{\rho}(0) H_I^2\right] = |00\rangle_{bc bc} \langle 00| Tr_a\left[\hat{\rho}_{th} H_I^2\right] \tag{6.27}$$

The Hamiltonian squared, H_I^2, has the form

$$\begin{aligned} H_I^2 = \frac{1}{V_b}\int_b d^3x \left(\hat{\Psi}_a(\vec{x})\,\hat{b}^\dagger + \hat{\Psi}_a^\dagger(\vec{x})\,\hat{b}\right) \int_b d^3x' \left(\hat{\Psi}_a(\vec{x}')\,\hat{b}^\dagger + \hat{\Psi}_a^\dagger(\vec{x}')\,\hat{b}\right) + \\ + \frac{1}{V_c}\int_c d^3x \left(\hat{\Psi}_a(\vec{x})\,\hat{c}^\dagger + \hat{\Psi}_a^\dagger(\vec{x})\,\hat{c}\right) \int_c d^3x' \left(\hat{\Psi}_a(\vec{x}')\,\hat{c}^\dagger + \hat{\Psi}_a^\dagger(\vec{x}')\,\hat{c}\right) + \\ + 2\frac{1}{\sqrt{V_b V_c}}\int_b d^3x \left(\hat{\Psi}_a(\vec{x})\,\hat{b}^\dagger + \hat{\Psi}_a^\dagger(\vec{x})\,\hat{b}\right) \int_c d^3x' \left(\hat{\Psi}_a(\vec{x}')\,\hat{c}^\dagger + \hat{\Psi}_a^\dagger(\vec{x}')\,\hat{c}\right). \end{aligned} \tag{6.28}$$

Substituting back to Eq.(6.27) and after disregarding those terms that contain the following zero quantities,

$$\left\langle \hat{\Psi}_a(\vec{x})\,\hat{\Psi}_a(\vec{x}') \right\rangle_{th} = \left\langle \hat{\Psi}_a^\dagger(\vec{x})\,\hat{\Psi}_a^\dagger(\vec{x}') \right\rangle_{th} = 0 \tag{6.29}$$

$$|00\rangle\langle 00|\,\hat{b}^\dagger\hat{b} = |00\rangle\langle 00|\,\hat{c}^\dagger\hat{c} = |00\rangle\langle 00|\,\hat{b}^\dagger\hat{c} = |00\rangle\langle 00|\,\hat{b}\hat{c}^\dagger = 0, \tag{6.30}$$

we find

$$A_3 = \left(\frac{1}{V_b} \int\limits_b d^3x \int\limits_b d^3x' \left\langle \hat{\Psi}_a^\dagger (\vec{x}) \, \hat{\Psi}_a (\vec{x}') \right\rangle_{th} + \right.$$
$$\left. + \frac{1}{V_c} \int\limits_c d^3x \int\limits_c d^3x' \left\langle \hat{\Psi}_a^\dagger (\vec{x}) \, \hat{\Psi}_a (\vec{x}') \right\rangle_{th} \right) |00\rangle \langle 00| \,. \quad (6.31)$$

Calculation of A_4 It can easily be seen that

$$A_4 = A_3. \quad (6.32)$$

Calculation of A_5

$$A_5 = Tr_a \left[H_I \hat{\rho}(0) \, H_I \right]$$
$$= Tr_a \left\{ \left[\frac{1}{\sqrt{V_b}} \int\limits_b d^3x \left(\hat{\Psi}_a (\vec{x}) \, \hat{b}^\dagger + \hat{\Psi}_a^\dagger (\vec{x}) \, \hat{b} \right) + \frac{1}{\sqrt{V_c}} \int\limits_c d^3x \left(\hat{\Psi}_a (\vec{x}) \, \hat{c}^\dagger + \hat{\Psi}_a^\dagger (\vec{x}) \, \hat{c} \right) \right] \otimes \right.$$
$$\otimes \hat{\rho}_{th} \otimes |00\rangle_{bc bc} \langle 00| \otimes \left[\frac{1}{\sqrt{V_b}} \int\limits_b d^3x' \left(\hat{\Psi}_a (\vec{x}') \, \hat{b}^\dagger + \hat{\Psi}_a^\dagger (\vec{x}') \, \hat{b} \right) + \right.$$
$$\left. \left. + \frac{1}{\sqrt{V_c}} \int\limits_c d^3x' \left(\hat{\Psi}_a (\vec{x}') \, \hat{c}^\dagger + \hat{\Psi}_a^\dagger (\vec{x}') \, \hat{c} \right) \right] \right\}$$

We get no contribution from those terms that contain,

$$\hat{b}|0\rangle_b = \hat{c}|0\rangle_c = {}_b\langle 0| \, \hat{b}^\dagger = {}_c\langle 0| \, \hat{c}^\dagger = 0.$$

The rest of the formula reads,

$$A_5 = \frac{1}{V_b} \int\limits_b d^3x \int\limits_b d^3x' \left\langle \hat{\Psi}_a^\dagger (\vec{x}') \, \hat{\Psi}_a (\vec{x}) \right\rangle_{th} \cdot \underbrace{\hat{b}^\dagger |00\rangle \langle 00| \, \hat{b}}_{|10\rangle\langle 10|} +$$
$$+ \frac{1}{V_c} \int\limits_c d^3x \int\limits_c d^3x' \left\langle \hat{\Psi}_a^\dagger (\vec{x}') \, \hat{\Psi}_a (\vec{x}) \right\rangle_{th} \cdot \underbrace{\hat{c}^\dagger |00\rangle \langle 00| \, \hat{c}}_{|01\rangle\langle 01|} +$$
$$+ \frac{1}{\sqrt{V_b V_c}} \int\limits_b d^3x \int\limits_c d^3x' \left\langle \hat{\Psi}_a^\dagger (\vec{x}') \, \hat{\Psi}_a (\vec{x}) \right\rangle_{th} \cdot \underbrace{\hat{b}^\dagger |00\rangle \langle 00| \, \hat{c}}_{|10\rangle\langle 01|} +$$
$$+ \frac{1}{\sqrt{V_c V_b}} \int\limits_c d^3x \int\limits_b d^3x' \left\langle \hat{\Psi}_a^\dagger (\vec{x}') \, \hat{\Psi}_a (\vec{x}) \right\rangle_{th} \cdot \underbrace{\hat{c}^\dagger |00\rangle \langle 00| \, \hat{b}}_{|01\rangle\langle 10|}.$$

At the last term we rename $x \leftrightarrow x'$, and since

$$\begin{aligned}\left\langle \hat{\Psi}_a^\dagger(\vec{x})\,\hat{\Psi}_a(\vec{x}')\right\rangle_{th} &= \sum_{k,k'} \varphi_k(\vec{x})\,\varphi_{k'}(\vec{x}')\left\langle \hat{a}_k^\dagger \hat{a}_{k'}\right\rangle_{th} \\ &= \sum_{k} \varphi_k(\vec{x})\,\varphi_k(\vec{x}')\left\langle \hat{a}_k^\dagger \hat{a}_k\right\rangle_{th} = \sum_{k} \varphi_k(\vec{x}')\varphi_k(\vec{x})\left\langle \hat{a}_k^\dagger \hat{a}_k\right\rangle_{th} \\ &= \left\langle \hat{\Psi}_a^\dagger(\vec{x}')\,\hat{\Psi}_a(\vec{x})\right\rangle_{th},\end{aligned} \tag{6.33}$$

the final form of the term A_5 reads

$$\begin{aligned}A_5 = \frac{1}{V_b}\int_b d^3x \int_b d^3x' \left\langle \hat{\Psi}_a^\dagger(\vec{x}')\,\hat{\Psi}_a(\vec{x})\right\rangle_{th} \cdot |10\rangle\langle 10| + \\ + \frac{1}{V_c}\int_c d^3x \int_c d^3x' \left\langle \hat{\Psi}_a^\dagger(\vec{x}')\,\hat{\Psi}_a(\vec{x})\right\rangle_{th} \cdot |01\rangle\langle 01| + \\ + \frac{1}{\sqrt{V_b V_c}}\int_b d^3x \int_c d^3x' \left\langle \hat{\Psi}_a^\dagger(\vec{x}')\,\hat{\Psi}_a(\vec{x})\right\rangle_{th} \cdot |10\rangle\langle 01| + \\ + \frac{1}{\sqrt{V_b V_c}}\int_b d^3x \int_c d^3x' \left\langle \hat{\Psi}_a^\dagger(\vec{x}')\,\hat{\Psi}_a(\vec{x})\right\rangle_{th} \cdot |01\rangle\langle 10|.\end{aligned} \tag{6.34}$$

Having calculated all the quantities A_i we substitute them in Eq.(6.19) and find the expression for the time-evolved reduced density matrix of the two quantum probes up to second order in Γ,

$$\begin{aligned}\hat{\rho}_{bc}(\delta t) = \left[1-\Gamma^2(I_{bb}+I_{cc})\right]\cdot|00\rangle\langle 00| + \Gamma^2 I_{bb}|10\rangle\langle 10| + \\ + \Gamma^2 I_{cc}|01\rangle\langle 01| + \Gamma^2 I_{bc}|10\rangle\langle 01| + \Gamma^2 I_{bc}|01\rangle\langle 10|,\end{aligned} \tag{6.35}$$

where

$$I_{ij} = \frac{1}{\sqrt{V_i V_j}}\int_i d^3x \int_j d^3x' \left\langle \hat{\Psi}_a^\dagger(\vec{x}')\,\hat{\Psi}_a(\vec{x})\right\rangle_{th}. \tag{6.36}$$

Now that we have the expression for the reduced quantum state of the probes Eq.(6.35) we can proceed and calculate an entanglement measure of the state in order to study the induced entanglement from the field to the probes. It should be emphasized at this point that the two probes were initially independent being in a product state while during the interaction they interacted locally only with the bosonic field and not with each other. We conclude that whatever entanglement we find in the state Eq.(6.35) it has originated from the spatial entanglement of the field's thermal state.

6.3 Convergence issues

Before we proceed to investigate the existence and amount of entanglement between the two quantum probes, we first have to elaborate on the convergence of the density matrix's perturbative expansion (6.35). We need to do that for two major reasons:

One reason is the condensation phenomenon, since the ground state is occupied be a huge number of particles and we will see below that $\left\langle \hat{\Psi}_a^\dagger(\vec{x}')\,\hat{\Psi}_a(\vec{x})\right\rangle_{th}$ and consequently $|I_{ij}|$ gets such large values that could completely destroy the convergence of (6.35). So we need to investigate the order of magnitude of every order Γ^n in the expansion and determine the parameters properly in order to achieve convergence.

A second reason is the weird factor $1/\sqrt{V_iV_j}$ in (6.36), which *seems* to ruin the convergence when $V_i \ll V$. In this section we are going to resolve these issues.

6.3.1 The behaviour of I_{ij}

The quantity I_{ij} is important not only because it plays a major role in the convergence of (6.35) but also, as we will see in later sections, because it's the quantity that solely determines the existence and amount of entanglement between the probes.

For that purpose we repeat its expression here for convenience,

$$I_{ij} = \frac{1}{\sqrt{V_iV_j}} \int\limits_i d^3x \int\limits_j d^3x' \left\langle \hat{\Psi}_a^\dagger(\vec{x}')\,\hat{\Psi}_a(\vec{x})\right\rangle_{th}. \tag{6.37}$$

For simplicity, in the subsequent analysis we assume that the probes occupy equal volume, i.e. $V_b = V_c$. By using the decomposition (6.23) for the field operator we get

$$I_{ij} = \frac{1}{V_i} \sum_k \left(\int\limits_i d^3x \varphi_k(\vec{x}) \right) \left(\int\limits_j d^3x' \varphi_k(\vec{x}') \right) \langle \hat{n}_k \rangle, \tag{6.38}$$

where $\langle \hat{n}_k \rangle = 1/\left(e^{\beta(E_k-\mu)}-1\right)$ the mean occupation number of the state $\varphi_k(\vec{x})$. We assume that the bosonic field is trapped inside a 3-dimensional cube of side length L and volume $V = L^3$ and find the one-particle Hamiltonian's eigenstates to be

$$\varphi_{\{n_i\}}(\vec{x}) = \sqrt{\frac{8}{V}} \sin\frac{n_1\pi x}{L} \sin\frac{n_2\pi y}{L} \sin\frac{n_3\pi z}{L}. \tag{6.39}$$

We substitute in (6.38) and after the evaluation of the integrals we find

$$I_{ij} = \frac{8}{V_iV} \sum_{n_1,n_2,n_3} A_i(n_1,n_2,n_3)\, A_j(n_1,n_2,n_3) \left\langle \hat{n}_{\{n_i\}} \right\rangle, \tag{6.40}$$

where

$$A_i(n_1,n_2,n_3) = \left(\int\limits_{x_{i1}}^{x_{i2}} dx \sin\frac{n_1\pi x}{L} \right) \cdot \left(\int\limits_{y_{i1}}^{y_{i2}} dy \sin\frac{n_2\pi y}{L} \right) \cdot \left(\int\limits_{z_{i1}}^{z_{i2}} dz \sin\frac{n_3\pi z}{L} \right). \tag{6.41}$$

At this point we want to find those parameters that determine the order of magnitute not only of the second order terms in (6.35) but also of the higher order terms, for every value of V_i/V not matter how small. In order to find the maximum value of I_{ij}, and hence its order of magnitude, we take advantage of the fact that

$$\left| \int\limits_{x_{i1}}^{x_{i2}} dx \sin\frac{n_1\pi x}{L} \right| = \frac{L}{n_1\pi} \left| \cos\frac{n_1\pi x_{i1}}{L} - \cos\frac{n_1\pi x_{i2}}{L} \right| \leq \frac{2L}{n_1\pi} \leq L, \tag{6.42}$$

which means that

$$|A_i(n_1,n_2,n_3)| \leq L^3 = V. \tag{6.43}$$

So, the maximum value of I_{ij} will be

$$\begin{aligned}
|I_{ij}| &= \frac{8}{V_i V} \left| \sum_{n_1,n_2,n_3} A_i(n_1,n_2,n_3) A_j(n_1,n_2,n_3) \left\langle \hat{n}_{\{n_i\}} \right\rangle \right| \\
&\leq \frac{8}{V_i V} \sum_{n_1,n_2,n_3} |A_i(n_1,n_2,n_3)| \cdot |A_j(n_1,n_2,n_3)| \left\langle \hat{n}_{\{n_i\}} \right\rangle \\
&\leq \frac{10V}{V_i} \sum_{n_1,n_2,n_3} \left\langle \hat{n}_{\{n_i\}} \right\rangle = 10\frac{V}{V_i} N \quad \Leftrightarrow \\
&\Leftrightarrow \quad |I_{ij}| \leq 10 \left(\frac{V}{V_i} \right) \rho V,
\end{aligned} \tag{6.44}$$

where $\rho = \frac{N}{V}$ is the density of the bosonic field (i.e. number of particles per unit volume). As long as V_i occupies a finite and not too small fraction of the total volume V, i.e.

$$2 \leq \frac{V}{V_i} \leq \text{some small number (e.g. 10)}, \tag{6.45}$$

then the order of magnitude of the maximum possible value of I_{ij} is determined by

$$|I_{ij}| \sim 10\rho V = 10N. \tag{6.46}$$

In this case the order of magnitude of the second order terms in the expansion of $\hat{\rho}_{bc}(\delta t)$, (6.35), is

$$OM(2) = 10\Gamma^2 N, \tag{6.47}$$

where we have denoted

$$\begin{aligned}
OM(2) = &\text{Order of magnitude of the} \\
&\text{2nd-order terms with respect to } \Gamma.
\end{aligned} \tag{6.48}$$

In this scenario, where (6.45) is satisfied, in order for the expansion (6.35) to converge we just have to demand the following condition,

$$OM(2) = 10\Gamma^2 N \ll 1, \tag{6.49}$$

and this can be satisfied quite easily (e.g. $\Gamma = 10^{-5}, N = 10^6$). So what we have learned is that the condensation phase of the bosonic gas doesn't actually create any problems in the convergence. In the analysis above, the condensation phase didn't appear explicitly because it wasn't necessary since our calculations, Eq. (6.44), hold for every temperature either $T > T_c$ or $T \leq T_c$.

Of course, if we want to make sure that the expansion converges we have to see how the higher order terms behave as well. However, we will not do this for this scenario because it's not realistic. The quantum probes cannot be of comparable volume to the total volume of the field!

Order of magnitude when $V_i \ll V$.

In realistic experimental settings, like the one we are going to discuss in a latter section, the volume each probe occupies is orders of magnitude smaller than V, satisfying

$$V_i \ll V. \tag{6.50}$$

At first glance, it seems that $|I_{ij}|$ blows up for $V_i \ll V$ but this is not the case if we look more carefully. In particular, let's examine a single integral of Eq. (6.41) and also assume for simplicity that

$$V_i \ll V \quad \Leftrightarrow \quad L_i \ll L, \tag{6.51}$$

where L_i is the side of the cube, occupied by probe i, with volume V_i. This assumption is harmless and it just says that all the three sides of the cube i are of the same order of magnitude. One of the integrals is

$$\int_{x_{i1}}^{x_{i2}} dx \sin\frac{n_1\pi x}{L} = \frac{L}{n_1\pi}\int_{\bar{x}_1}^{\bar{x}_2} d\bar{x}\sin\bar{x}, \tag{6.52}$$

where $\bar{x}_a = \frac{n_1\pi x_{ia}}{L}$. Since

$$L_i = x_{i2} - x_{i1} \approx y_{i2} - y_{i1} \approx z_{i2} - z_{i1}, \tag{6.53}$$

and $L_i \ll L$, it approximately holds that

$$\bar{x}_2 - \bar{x}_1 = n_1\pi\frac{x_{i2} - x_{i1}}{L} \ll 1, \tag{6.54}$$

which means that the variable $\bar{x}$ in (6.52) varies negligibly since the limits of the integral are almost equal. Taking advantage of this fact, we can approximate the sinus by it's taylor expansion about the point $\bar{x} = \bar{x}_1$ and keep terms only up to first order, i.e.

$$\sin\bar{x} \approx (\bar{x} - \bar{x}_1)\cos\bar{x}_1 + \sin\bar{x}_1, \tag{6.55}$$

and consequently

$$\begin{aligned}\int_{x_{i1}}^{x_{i2}} dx \sin\frac{n_1\pi x}{L} = \frac{L}{n_1\pi}\int_{\bar{x}_1}^{\bar{x}_2} d\bar{x}\sin\bar{x} &\approx \frac{L}{n_1\pi}(\bar{x}_2 - \bar{x}_1)\sin\bar{x}_1 \\ &= (x_{i2} - x_{i1})\sin\frac{n_1\pi x_{i1}}{L}.\end{aligned} \tag{6.56}$$

We do the same approximations for the other two dimension y, z and substituting back to (6.41) we get,

$$\begin{aligned}A_i(n_1, n_2, n_3) &\approx (x_{i2} - x_{i1})(y_{i2} - y_{i1})(z_{i2} - z_{i1})\sin\frac{n_1\pi x_{i1}}{L}\sin\frac{n_2\pi y_{i1}}{L}\sin\frac{n_3\pi z_{i1}}{L} \\ &= V_i \cdot \sin\frac{n_1\pi x_{i1}}{L}\sin\frac{n_2\pi y_{i1}}{L}\sin\frac{n_3\pi z_{i1}}{L}.\end{aligned} \tag{6.57}$$

where

$$V_i = (x_{i2} - x_{i1})(y_{i2} - y_{i1})(z_{i2} - z_{i1}). \tag{6.58}$$

After using these approximations, I_{ij} turns out to have the following form

$$I_{ij} = V_i \sum_{n_1,n_2,n_3} \varphi_{(n_1,n_2,n_3)}\left(\vec{x}_{i_1}\right) \varphi_{(n_1,n_2,n_3)}\left(\vec{x}_{j_1}\right) \left\langle \hat{n}_{(n_1,n_2,n_3)} \right\rangle_{th}, \tag{6.59}$$

so the maximum value of $|I_{ij}|$ becomes

$$\begin{aligned} |I_{ij}| &\leq V_i \sum_{n_1,n_2,n_3} \left|\varphi_{(n_1,n_2,n_3)}\left(\vec{x}_{i_1}\right)\right| \cdot \left|\varphi_{(n_1,n_2,n_3)}\left(\vec{x}_{j_1}\right)\right| \left\langle \hat{n}_{(n_1,n_2,n_3)} \right\rangle \\ &\leq \frac{10N}{V} V_i = 10\rho V_i. \end{aligned} \tag{6.60}$$

We conclude that the order of magnitude -or, to be more precise, the maximum value possible- of the second order terms in (6.35) is

$$OM(2) = 10\Gamma^2 \rho V_i, \tag{6.61}$$

where $\rho = N/V$ and the notation is explained in (6.48).

Before we make any comments on this relation, we will proceed to find the order of magnitude of higher order terms in Γ, i.e. $OM(2n)$. Note that the exponent of Γ always has to be an even number, hence the notation $2n$, because the odd powers give no contribution due to the unequal number of $\hat{\Psi}_a\left(\vec{x}\right)$ and $\hat{\Psi}_a^\dagger\left(\vec{x}'\right)$ involved in the means values of the form $\left\langle \cdots \hat{\Psi}_a^\dagger\left(\vec{x}'\right) \cdots \hat{\Psi}_a\left(\vec{x}\right) \cdots \right\rangle_{th}$. By examining carefully the equations (6.18), (6.19) we can see that the following type of terms of order $\mathrm{O}\left(\Gamma^{2n}\right)$ participate,

$$\begin{gathered} \Gamma^{2n} Tr_a \left[\hat{\rho}\left(0\right) \hat{H}_I^{2n}\right], \quad \Gamma^{2n} Tr_a \left[\hat{H}_I^{2n} \hat{\rho}\left(0\right)\right] \\ \Gamma^{2n} Tr_a \left[\hat{H}_I^{m} \hat{\rho}\left(0\right) \hat{H}_I^{2n-m}\right], \quad \Gamma^{2n} Tr_a \left[\hat{H}_I^{2n-m} \hat{\rho}\left(0\right) \hat{H}_I^{m}\right], \end{gathered} \tag{6.62}$$

for every $m < 2n$. Now, notice that whether $\hat{H}_I$ is located at the left or right side of $\hat{\rho}\left(0\right)$ is unrelated to the magnitude of that term. The relative position of $\hat{H}_I$ and $\hat{\rho}\left(0\right)$ only determines which vectors $|ij\rangle_{bc}$ will participate. The only thing that determines the magnitude of the coefficients is the total number of left and right Hamiltonians, which is always $2n$, i.e. $\hat{H}_I^{2n}$. In order to understand the following point better, let's see what happened in the case when the total number of Hamiltonians was $\hat{H}_I^2$. Every coefficient, e.g. see (6.31) and (6.34), involves two volume integrals of the one-particle wavefunction just like in (6.38) and a coefficient $1/V_i$. Now that our order is increased by n, i.e. we have $\hat{H}_I^{2n}$ Hamiltonians, the corresponding coefficients will involve $2n$ volume integrals and a coefficient

$$1/V_i^n. \tag{6.63}$$

Every volume integral

$$\sqrt{\frac{8}{V}} \left(\int_{x_{i1}}^{x_{i2}} dx \sin\frac{n_1 \pi x}{L}\right) \cdot \left(\int_{y_{i1}}^{y_{i2}} dy \sin\frac{n_2 \pi y}{L}\right) \cdot \left(\int_{z_{i1}}^{z_{i2}} dz \sin\frac{n_3 \pi z}{L}\right)$$

contributes a maximum magnitude of $V_i\sqrt{10/V}$ in the $V_i \ll V$ approximation, as see by (**??**), which means that the total of $2n$ volume integrals will contribute a coefficient of maximum magnitude

$$\left(V_i\sqrt{10/V}\right)^{2n} = 10^n V_i^{2n}/V^n. \tag{6.64}$$

The only thing left to consider is the sum over $2n$ sets of quantum numbers (n_1, n_2, n_3) of mean values of the form

$$\left\langle \cdots \hat{a}^{\dagger}_{\{n_i\}} \cdots \hat{a}_{\{n_i\}} \cdots \right\rangle_{th}, \tag{6.65}$$

just like in (6.44) in the case of 2nd order. The operators $\left\{\hat{a}^{\dagger}_{\{n_i\}}, \hat{a}_{\{n_i\}}\right\}$ are the energy modes, i.e. the create and destroy particles with wavefunction (6.39) and quantum numbers (n_1, n_2, n_3). There are equal number of creation and annihilation operators in the mean value (6.65) in order to get a non-zero result. This sum will yield the following maximum value possible,

$$\begin{aligned} \sum_{2n-sets\ of\ \{n_i\}} & \left[\left\langle \cdots \hat{a}^{\dagger}_{\{n_i\}} \cdots \hat{a}_{\{n'_i\}} \cdots \right\rangle_{th} + (all\ possible\ permutations)\right] = \\ & = c_n N^n + c_{n-1} N^{n-1} + \ldots + c_1 N^1 + c_0 \\ & \sim N^n, \end{aligned} \tag{6.66}$$

where the last equation gives the order of magnitude of the sum, i.e. N^n for $N \gg 1$, and we also assumed that all the particles occupy the ground state in order to get the maximum result. Note that (6.66) holds only for small n, e.g. $n = 2$, since for large n the coefficient c_n may be larger than unity. Of course, the point is not to prove the convergence of the perturbation series for arbitrary n since such a task may be impossible after all, the series may be asymptotic. At this point we only care to find the necessary condition for small n, corresponding to terms that we will actually use in the calculations.

If we put all these factors together by multiplying (6.63), (6.64) and (6.66 we get the total order of magnitude of the terms corresponding to $\Gamma^2 n$, i.e.

$$OM(2n) = \left(10\Gamma^2 \rho V_i\right)^n, \tag{6.67}$$

which agrees with (6.61) for $n = 1$. This last equation achieves the desired convergence (for small n), since by choosing properly the parameters so that

$$10\Gamma^2 \rho V_i \ll 1 \tag{6.68}$$

the contribution of higher order terms will be negligible. For large n, (6.68) is not applicable.

6.4 Short review of the entanglement measures to be used

In this section we will review two of the most famous and easily computable entanglement measures, the negativity and concurrence, before we go on and apply them to the reduced quantum state of the two probes. For a more detailed discussion on entanglement measures, see Section 2.8 of *Part II*.

6.4.1 Negativity

Negativity is an entanglement measure first introduced in [95] and is based on the *Positive Partial Transpose* (PPT) criterion [44]. According to the PPT criterion if a density matrix is of separable form, i.e.

$$\hat{\rho}_{bc} = \sum_i p_i \hat{\rho}_{ib} \otimes \hat{\rho}_{ic}, \tag{6.69}$$

then by taking the partial transpose of the state, which means to take the total transpose only of one of the subsystems in the basis of interest,

$$\hat{\rho}_{bc}^{PT} = \sum_i p_i \hat{\rho}_{ib} \otimes \hat{\rho}_{ic}^{T} \tag{6.70}$$

then $\hat{\rho}_{bc}^{PT}$ is a well-defined density matrix with non-negative eigenvalues, since $\hat{\rho}_{ic}^{T}$ itself is a well-defined density matrix after a total transposition. We conclude that if the quantum state is of the separable form Eq.(6.69) then its partial transpose Eq.(6.70) has non-negative eigenvalues. On the other hand, if the state $\hat{\rho}_{bc}$ is entangled then its partial transpose may have negative eigenvalues.

Horodecki *et. al.* [45] proved that for bipartite systems with Hilbert space dimensions 2×2 and 2×3 the PPT criterion is necessary and sufficient. In our case, the Hilbert space dimension of the quantum probes Eq.(6.1) is 2×2, which means that if $\hat{\rho}_{bc}$ is entangled then $\hat{\rho}_{bc}^{PT}$ *will* have negative eigenvalues while if it's separable then the eigenvalues of $\hat{\rho}_{bc}^{PT}$ will be only non-negative.

The Negativity of a quantum state is defined as the absolute value of the sum of the negative eigenvalues of its partial transposed state. If we denote with λ_i the negative eigenvalues of $\hat{\rho}_{bc}^{PT}$ then

$$N\left(\hat{\rho}_{bc}\right) = \left| \sum_i \lambda_i \right|. \tag{6.71}$$

6.4.2 Concurrence

Concurrence, $C\left(\hat{\rho}_{bc}\right)$, was first introduced by Wooters [97]. Its popularity stems from the fact that for two qubits it's directly related to the -hard to compute- entanglement measure *Entanglement of Formation* $E_F\left(\hat{\rho}_{bc}\right)$ in the closed form

$$E_F\left(\hat{\rho}_{bc}\right) = H\left(\frac{1+\sqrt{1-C(\hat{\rho}_{bc})^2}}{2}\right), \tag{6.72}$$

where

$$H\left(p\right) = -p\log p - \left(1-p\right)\log\left(1-p\right).$$

The concurrence $C\left(\hat{\rho}_{bc}\right)$ is given by,

$$C\left(\hat{\rho}_{bc}\right) = \max\left\{0, \sqrt{R_1} - \sqrt{R_2} - \sqrt{R_3} - \sqrt{R_4}\right\} \tag{6.73}$$

where the R_i are the decreasingly ordered eigenvalues of the matrix

$$R = \hat{\rho}_{bc}\sigma_y \otimes \sigma_y \hat{\rho}_{bc}^{*} \sigma_y \otimes \sigma_y \tag{6.74}$$

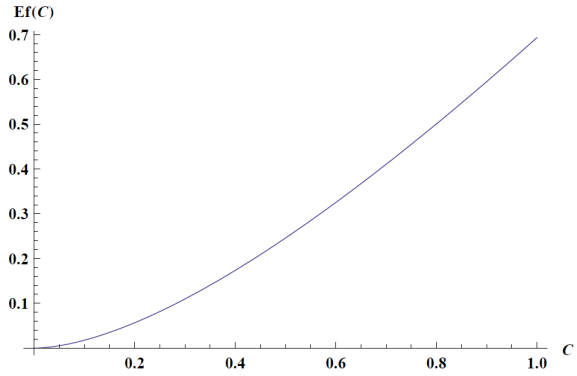

Figure 6.1: The dependence of the *Entanglement of Formation* $E_F(\hat{\rho}_{bc})$ to the *Concurrence* $C(\hat{\rho}_{bc})$

.

and σ_y is the second Pauli matrix. Since R is hermitian, regardless of the state's separability, the eigenvalues R_i are non-negative while it can be proved that

$$0 \leq C(\hat{\rho}_{bc}) \leq 1. \tag{6.75}$$

It's straightforward to see from (6.72) that the Entanglement of Formation is maximized as $C(\hat{\rho}_{bc}) \to 1$ which gives $C(\hat{\rho}_{bc})$ the meaning of an entanglement measure itself. We can see this behaviour in Figure 6.1, where we see the dependence of $E_F(\hat{\rho}_{bc})$ to $C(\hat{\rho}_{bc})$.

6.5 Calculation of Negativity

In order to calculate the negativity $N(\hat{\rho}_{bc})$ we first need to take the partial transpose of the state. We choose to transpose the state of the second subsystem, the quantum probe c, namely

$$_{bc}\langle ij|\,\hat{\rho}_{bc}|km\rangle_{bc} \to {}_{bc}\langle im|\,\hat{\rho}_{bc}|kj\rangle_{bc}. \tag{6.76}$$

Note that we could also transpose the first subsystem, it makes no difference.

Now, the partial transposed state $\hat{\rho}_{bc}^{PT}$ reads

$$\begin{aligned}\hat{\rho}_{bc}^{PT}(\delta t) = \left[1-\Gamma^2(I_{bb}+I_{cc})\right]\cdot|00\rangle\langle 00| + \Gamma^2 I_{bb}\,|10\rangle\langle 10| + \\ + \Gamma^2 I_{cc}\,|01\rangle\langle 01| + \Gamma^2 I_{bc}\,|11\rangle\langle 00| + \Gamma^2 I_{bc}\,|00\rangle\langle 11|,\end{aligned} \tag{6.77}$$

where the following changes occured,

$$|10\rangle\langle 01| \to |11\rangle\langle 00|, \quad |01\rangle\langle 10| \to |00\rangle\langle 11|. \tag{6.78}$$

It's useful to right down the matrix form of the states $\hat{\rho}_{bc}, \hat{\rho}_{bc}^{PT}$. We choose the following

matrix representation,

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
$$|00\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad |11\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{6.79}$$
$$|01\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |10\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}.$$

In this representation, the quantum states (6.35) and (6.77) have the following matrix forms,

$$\hat{\rho}_{bc}(\delta t) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \Gamma^2 I_{bb} & \Gamma^2 I_{bc} & 0 \\ 0 & \Gamma^2 I_{bc} & \Gamma^2 I_{cc} & 0 \\ 0 & 0 & 0 & 1-C \end{pmatrix} \tag{6.80}$$

and

$$\hat{\rho}_{bc}^{PT}(\delta t) = \begin{pmatrix} 0 & 0 & 0 & \Gamma^2 I_{bc} \\ 0 & \Gamma^2 I_{bb} & 0 & 0 \\ 0 & 0 & \Gamma^2 I_{cc} & 0 \\ \Gamma^2 I_{bc} & 0 & 0 & 1-C \end{pmatrix}, \tag{6.81}$$

where

$$C = \Gamma^2 (I_{bb} + I_{cc}) \tag{6.82}$$

and $I_{ij} = \frac{1}{\sqrt{V_i V_j}} \int\limits_i d^3x \int\limits_j d^3x' \left\langle \hat{\Psi}_a^\dagger(\vec{x}') \hat{\Psi}_a(\vec{x}) \right\rangle_{th}$. Notice that the normalization $Tr\hat{\rho}_{bc}(\delta t) = 1$ still holds up to second order in Γ after our approximation of small duration of the interaction.

Now, we can easily find the eigenvalues λ_i of the partially transposed state $\hat{\rho}_{bc}^{PT}$ to be

$$\lambda_1 = \Gamma^2 I_{bb} \geq 0 \tag{6.83}$$
$$\lambda_2 = \Gamma^2 I_{cc} \geq 0 \tag{6.84}$$
$$\lambda_3 = \frac{1}{2}\left(1 - C + \sqrt{(1-C)^2 + 4\Gamma^4 I_{bc}^2}\right) \geq 0 \tag{6.85}$$
$$\lambda_4 = \frac{1}{2}\left(1 - C - \sqrt{(1-C)^2 + 4\Gamma^4 I_{bc}^2}\right) \leq 0. \tag{6.86}$$

The first two eigenvalues, λ_1 and λ_2, are positive and this is easy to check by looking at

I_{ij} Eq.(6.36) for $i=j$,

$$\begin{aligned} I_{ii} &= \frac{1}{V_i}\int\limits_i d^3x \int\limits_i d^3x' \left\langle \hat{\Psi}_a^{\dagger}\left(\vec{x}'\right)\hat{\Psi}_a\left(\vec{x}\right)\right\rangle_{th} \\ &= \frac{1}{V_i}\int\limits_i d^3x \int\limits_i d^3x' \sum_k \varphi_k\left(\vec{x}'\right)\varphi_k\left(\vec{x}\right)\langle\hat{n}_k\rangle = \frac{1}{V_i}\sum_k \left(\int\limits_i d^3x \varphi_k\left(\vec{x}\right)\right)^2 \langle\hat{n}_k\rangle \\ &\geq 0. \end{aligned} \tag{6.87}$$

The important eigenvalue is λ_4, which is negative for every $I_{bc}\neq 0$, while it's zero for $I_{bc}=0$. According to the definition of negativity Eq.(6.71) we find the following formula

$$\begin{aligned} N\left[\hat{\rho}_{bc}\left(\delta t\right)\right] &= \left|\lambda_4\right| \\ &= \frac{1}{2}\left(\sqrt{\left(1-C\right)^2+4\Gamma^4 I_{bc}^2}-\left(1-C\right)\right) \\ &= \mathrm{I}_{bc}^2\Gamma^4 + O\left(\Gamma^5\right). \end{aligned} \tag{6.88}$$

Notice the Γ^4 factor. In our perturbative expansion, we kept terms only up to second order Γ^2 and considered the Γ^4 terms to be negligible. However, the Γ^4-order terms may contribute to the formula (6.88) and change the result since it's of the same order of magnitude! So, we are forced to calculate the contribution of the Γ^4 terms in the formula of negativity by going back in the perturbative expansion (6.18). This will be done in the next section.

6.5.1 Taking into account the 4^{rth}-order terms

We first need to see how will the reduced density matrix of the probes be modified.We repeat here the perturbative expansion for convenience including the relevant higher order terms,

$$\begin{aligned} \hat{\rho}\left(\delta t\right) &= Tr_a\left[\hat{U}\left(\delta t\right)\hat{\rho}\left(0\right)\hat{U}^{\dagger}\left(\delta t\right)\right] \\ &= Tr_a\left[\left(1-i\Gamma\hat{H}_I-\frac{\Gamma^2}{2}\hat{H}_I^2+i\frac{\Gamma^3}{3!}\hat{H}_I^3+\frac{\Gamma^4}{4!}\hat{H}_I^4+\mathrm{O}\left(\Gamma^5\right)\right)\otimes\hat{\rho}\left(0\right)\otimes \right. \\ &\qquad \left.\otimes\left(1+i\Gamma\hat{H}_I-\frac{\Gamma^2}{2}\hat{H}_I^2-i\frac{\Gamma^3}{3!}\hat{H}_I^3+\frac{\Gamma^4}{4!}\hat{H}_I^4+\mathrm{O}\left(\Gamma^5\right)\right)\right]. \end{aligned} \tag{6.89}$$

The extra 4^{rth} order terms, whose contribution we need to take into account, are the following,

$$\begin{aligned} \mathrm{B}_1 = Tr_a\left[\hat{H}_I\hat{\rho}\left(0\right)\hat{H}_I^3\right],\ \mathrm{B}_2 = Tr_a\left[\hat{H}_I^3\hat{\rho}\left(0\right)\hat{H}_I\right],\ \mathrm{B}_3 = Tr_a\left[\hat{H}_I^4\hat{\rho}\left(0\right)\right], \\ \mathrm{B}_4 = Tr_a\left[\hat{\rho}\left(0\right)\hat{H}_I^4\right],\ \mathrm{B}_5 = Tr_a\left[\hat{H}_I^2\hat{\rho}\left(0\right)\hat{H}_I^2\right]. \end{aligned} \tag{6.90}$$

This seems to be a really difficult task since the Hamiltonians are of high order and the calculations seem to be impossible. However this is not the case if we make our analysis

in the following clever way. First of all, by inspection we find that the terms B_1, B_2, B_3 and B_4 contribute only to the following -and existing- matrix elements

$$|10\rangle_{bc}\langle 10|\,,\ |01\rangle_{bc}\langle 01|\,,\ |10\rangle_{bc}\langle 01|\,,\ |01\rangle_{bc}\langle 10|\,, \tag{6.91}$$

while only B_5 contributes in all the elements (6.91) *plus* in the non-existing element $|11\rangle_{bc}\langle 11|$. We recall that the probes' state up to 2^{nd}-order is

$$\hat{\rho}_{bc}(\delta t) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \Gamma^2 I_{bb} & \Gamma^2 I_{bc} & 0 \\ 0 & \Gamma^2 I_{bc} & \Gamma^2 I_{cc} & 0 \\ 0 & 0 & 0 & 1-C \end{pmatrix}$$

. To make our arguments more clear, we have just argued that:

- None of the $B_1, B_2, B_3, B_4,$ contribute to the zero elements of the density matrix.
- Only B_5 contributes to the zero element "11" of the density matrix.
- All $B_1 - B_5,$ contribute to the existing non-zero elements of the density matrix.

Taking these remarks into account, the state up to 4^{rth} order will be

$$\hat{\rho}_{bc}(\delta t) = \begin{pmatrix} \Gamma^4 b_{11} & 0 & 0 & 0 \\ 0 & \Gamma^2 I_{bb} + \Gamma^4 a_{22} & \Gamma^2 I_{bc} + \Gamma^4 a_{23} & 0 \\ 0 & \Gamma^2 I_{bc} + \Gamma^4 a_{32} & \Gamma^2 I_{cc} + \Gamma^4 a_{33} & 0 \\ 0 & 0 & 0 & 1 - \Gamma^2 (I_{bb} + I_{cc}) + \Gamma^4 a_{44} \end{pmatrix}, \tag{6.92}$$

where we see the contribution a_{ij} from all the B_i terms and the *important* contribution $b_1 1$ coming only from the B_5 term. Why this contribution is important will be obvious in a while. At the moment we don't need to calculate all these contribution, we first have to see which of all these actually contribute to the negativity. The partially transposed state will be

$$\hat{\rho}_{bc}^{PT}(\delta t) = \begin{pmatrix} \Gamma^4 b_{11} & 0 & 0 & \Gamma^2 I_{bc} + \Gamma^4 a_{23} \\ 0 & \Gamma^2 I_{bb} + \Gamma^4 a_{22} & 0 & 0 \\ 0 & 0 & \Gamma^2 I_{cc} + \Gamma^4 a_{33} & 0 \\ \Gamma^2 I_{bc} + \Gamma^4 a_{32} & 0 & 0 & 1 - C + \Gamma^4 a_{44} \end{pmatrix}, \tag{6.93}$$

the eigenvalues of which are

$$\lambda'_1 = \Gamma^2 \mathrm{I}_{bb} + \Gamma^4 a_{22} \geq 0, \tag{6.94}$$

$$\lambda'_2 = \Gamma^2 \mathrm{I}_{cc} + \Gamma^4 a_{33} \geq 0, \tag{6.95}$$

$$\begin{aligned} \lambda'_3 = \frac{1}{2}\Big(1 + \Gamma^4 a_{11} + \Gamma^4 a_{44} - \Gamma^2 \mathrm{I}_{bb} - \Gamma^2 \mathrm{I}_{cc} + \sqrt{(-1 - \Gamma^4 a_{11} - \Gamma^4 a_{44} + \\ + \Gamma^2 \mathrm{I}_{bb} + \Gamma^2 \mathrm{I}_{cc})^2 - 4\left(\Gamma^4 a_{11} - \Gamma^8 a_{23} a_{32} + \Gamma^8 a_{11} a_{44} - \Gamma^6 a_{11} \mathrm{I}_{bb} - \right.} \\ \left. - \Gamma^6 a_{23} \mathrm{I}_{bc} - \Gamma^6 a_{32} \mathrm{I}_{bc} - \Gamma^4 \mathrm{I}_{bc}^2 - \Gamma^6 a_{11} \mathrm{I}_{cc})\right)} \Big) \approx \\ \approx 1 + (-\mathrm{I}_{bb} - \mathrm{I}_{cc})\,\Gamma^2 + \left(a_{44} + \mathrm{I}_{bc}^2\right)\Gamma^4 \geq 0, \end{aligned} \tag{6.96}$$

$$\lambda'_4 = \frac{1}{2}\Big(1+\Gamma^4 a_{11}+\Gamma^4 a_{44}-\Gamma^2 \mathrm{I}_{bb}-\Gamma^2 \mathrm{I}_{cc}-\sqrt{(-1-\Gamma^4 a_{11}-\Gamma^4 a_{44}+ \\ +\Gamma^2 \mathrm{I}_{bb}+\Gamma^2 \mathrm{I}_{cc})^2-4\left(\Gamma^4 a_{11}-\Gamma^8 a_{23}a_{32}+\Gamma^8 a_{11}a_{44}-\Gamma^6 a_{11}\mathrm{I}_{bb}- \\ -\Gamma^6 a_{23}\mathrm{I}_{bc}-\Gamma^6 a_{32}\mathrm{I}_{bc}-\Gamma^4 \mathrm{I}_{bc}^2-\Gamma^6 a_{11}\mathrm{I}_{cc}\right)}\Big) \approx \\ \approx (b_{11}-\mathrm{I}_{bc}^2)\Gamma^4. \tag{6.97}$$

We see how rapidly these expressions got simplified when we kept only the Γ_4 contributions and got rid of the higher orders. Three of the eigenvalues turn out to be always positive, i.e.

$$\lambda'_1,\ \lambda'_2,\ \lambda'_3\ \geq 0, \tag{6.98}$$

while only λ'_4 has the potential of being negative

$$\lambda'_4 = (b_{11}-\mathrm{I}_{bc}^2)\Gamma^4. \tag{6.99}$$

Admire the remarkable simplification! Of all those contributions in the density matrix only one of them, b_{11}, gives a correction to the negativity of order Γ^4! We remind that b_{11} is the contribution of the B_5 in the $|11\rangle_{bc}\langle 11|$ of the density matrix. The correct formula for the *Negativity* is now given by,

$$N' = \left(\mathrm{I}_{bc}^2 - b_{11}\right)\Gamma^4, \quad \text{only if} \quad \mathrm{I}_{bc}^2 \geq b_{11}. \tag{6.100}$$

We conclude that entanglement will exist only if $\mathrm{I}_{bc}^2 > b_{11}$, while if it's $b_{11} > \mathrm{I}_{bc}^2$ the eigenvalue λ'_4 will be positive and the quantum state of the probes will be separable. Also notice that if $b_{11} < 0$ then the quantum state will be entangled for every $|I_{bc}| > 0$, just like in the *old* (and insufficient) formula (6.88). What we have to do is to calculate the quantity b_{11}.

Calculation of b_{11}

We remind that b_{11} is the contribution of the

$$\frac{1}{4} Tr_a\left[\hat{H}_I^2 \hat{\rho}\,(0)\,\hat{H}_I^2\right] \tag{6.101}$$

term in the $|11\rangle_{bcbc}\langle 11|$ element of the density matrix. Recall the form of $\hat{H}_I^2$ which we calculated in (6.28). They only term of $\hat{H}_I^2$ that contributes is

$$\hat{H}_I^2 \to \frac{2}{V_i}\int\limits_b d^3x\left(\hat{\psi}_\alpha(\vec{x})\,\hat{b}^\dagger + \hat{\psi}_\alpha^\dagger(\vec{x})\,\hat{b}\right)\cdot\int\limits_c d^3x'\left(\hat{\psi}_\alpha(\vec{x}')\,\hat{c}^\dagger + \hat{\psi}_\alpha^\dagger(\vec{x}')\,\hat{c}\right), \tag{6.102}$$

since we want the combination of $\hat{b}^\dagger\hat{c}^\dagger$ and $\hat{b}\hat{c}$ in order to create the $|11\rangle_{bcbc}\langle 11| = \hat{b}^\dagger\hat{c}^\dagger|00\rangle_{bcbc}\langle 00|\,\hat{b}\hat{c}$ element. In more detail,

$$\hat{H}_I^2\hat{\rho}_{th}|00\rangle_{bc} \to \frac{2}{V_i}\int\limits_b d^3x_b\int\limits_c d^3x_c\hat{\psi}_\alpha(\vec{x}_b)\,\hat{\psi}_\alpha(\vec{x}_c)\,\hat{\rho}_{th}\cdot\overbrace{\hat{b}^\dagger\hat{c}^\dagger|00\rangle_{bc}}^{|11\rangle_{bc}} \tag{6.103}$$

$$_{bc}\langle 00|\,\hat{H}_I^2 \to \frac{2}{V_i}\int\limits_b d^3x'_b\int\limits_c d^3x'_c\hat{\psi}_\alpha^\dagger(\vec{x}'_b)\,\hat{\psi}_\alpha^\dagger(\vec{x}'_c)\cdot\underbrace{{}_{bc}\langle 00|\,\hat{b}\hat{c}}_{{}_{bc}\langle 11|}. \tag{6.104}$$

So, b_{11} will be

$$\begin{aligned} b_{11} &= \frac{1}{4}{}_{bc}\left\langle 11\right| Tr_a\left[\hat{H}_I^2\hat{\rho}\left(0\right)\hat{H}_I^2\right]\left|11\right\rangle_{bc} \\ &= \frac{1}{V_i^2}\int\limits_b d^3x_b\int\limits_c d^3x_c\int\limits_b d^3x'_b\int\limits_c d^3x'_c\ Tr_a\left[\hat{\rho}_{th}\hat{\psi}_\alpha^\dagger\left(\vec{x}'_b\right)\hat{\psi}_\alpha^\dagger\left(\vec{x}'_c\right)\hat{\psi}_\alpha\left(\vec{x}_b\right)\hat{\psi}_\alpha\left(\vec{x}_c\right)\right]. \end{aligned} \tag{6.105}$$

Using the decomposition $\hat{\psi}_\alpha\left(\vec{x}\right)=\sum\limits_{\vec{n}}\varphi_{\vec{n}}\left(\vec{x}\right)\hat{a}_{\vec{n}}$ for the field operator, following the notation $\vec{n}=(n_1,n_2,n_3)$ and $\sum\limits_{\vec{n}}\equiv\sum\limits_{n_1,n_2,n_3}$, we get

$$\begin{aligned} b_{11} = \frac{1}{V_i^2}\sum_{\vec{n}_b,\vec{n}_c,\vec{n}'_b,\vec{n}'_c}&\left(\int\limits_b d^3x_b\varphi_{\vec{n}_b}\left(\vec{x}_b\right)\right)\left(\int\limits_c d^3x_c\varphi_{\vec{n}_c}\left(\vec{x}_c\right)\right)\times \\ &\times\left(\int\limits_b d^3x'_b\varphi_{\vec{n}'_b}\left(\vec{x}'_b\right)\right)\left(\int\limits_c d^3x'_c\varphi_{\vec{n}'_c}\left(\vec{x}'_c\right)\right)\ Tr_a\left[\hat{\rho}_{th}\hat{a}_{\vec{n}'_b}^\dagger\hat{a}_{\vec{n}'_c}^\dagger\hat{a}_{\vec{n}_b}\hat{a}_{\vec{n}_c}\right]. \end{aligned} \tag{6.106}$$

Next we use the approximations (6.51), (6.56) corresponding to $V_i \ll V$ which just say that

$$\int\limits_i d^3x_i\varphi_{\vec{n}_i}\left(\vec{x}_i\right)\approx V_i\varphi_{\vec{n}_i}\left(\vec{x}_{i1}\right), \tag{6.107}$$

i.e. the wavefunction $\varphi_{\vec{n}_i}\left(\vec{x}_i\right)$ is almost constant inside the probe's volume, simplifying the expression to

$$b_{11}=V_i^2\sum_{\vec{n}_b,\vec{n}_c,\vec{n}'_b,\vec{n}'_c}\varphi_{\vec{n}_b}\left(\vec{x}_{b_1}\right)\varphi_{\vec{n}_c}\left(\vec{x}_{c_1}\right)\varphi_{\vec{n}'_b}\left(\vec{x}_{b_1}\right)\varphi_{\vec{n}'_c}\left(\vec{x}_{c_1}\right)\left\langle\hat{a}_{\vec{n}'_b}^\dagger\hat{a}_{\vec{n}'_c}^\dagger\hat{a}_{\vec{n}_b}\hat{a}_{\vec{n}_c}\right\rangle_{th}. \tag{6.108}$$

Before we substitute everything back in the formula of negativity, we need to explicitly calculate the mean value $\left\langle\hat{a}_{\vec{n}'_b}^\dagger\hat{a}_{\vec{n}'_c}^\dagger\hat{a}_{\vec{n}_b}\hat{a}_{\vec{n}_c}\right\rangle_{th}$.

Calculation of the mean value $\left\langle\hat{a}_{\vec{n}'_b}^\dagger\hat{a}_{\vec{n}'_c}^\dagger\hat{a}_{\vec{n}_b}\hat{a}_{\vec{n}_c}\right\rangle_{th}$

The thermal state can be decomposed as,

$$\begin{aligned} \hat{\rho}_{th} &= \frac{1}{Z}\exp\left[-\beta\sum_i\left(E_{\vec{n}_i}-\mu\right)\hat{a}_{\vec{n}_i}^\dagger\hat{a}_{\vec{n}_i}\right] \\ &= \sum_{N_{\vec{n}_1},N_{\vec{n}_2},\ldots}P_{\left\{N_{\vec{n}_i}\right\}}\left|N_{\vec{n}_1},N_{\vec{n}_2},\ldots\right\rangle\left\langle N_{\vec{n}_1},N_{\vec{n}_2},\ldots\right|, \end{aligned} \tag{6.109}$$

where

$$P_{\left\{N_{\vec{n}_i}\right\}}=\frac{1}{Z}\exp\left[-\beta\sum_i\left(E_{\vec{n}_i}-\mu\right)N_{\vec{n}_i}\right],\ \left(\sum_{N_{\vec{n}_1},N_{\vec{n}_2},\ldots}P_{\left\{N_{\vec{n}_i}\right\}}=1\right) \tag{6.110}$$

is the probability of having $N_{\vec{n}_1}$ particles in the single-particle state $\varphi_{\vec{n}_1}(\vec{x})$, $N_{\vec{n}_2}$ particles in $\varphi_{\vec{n}_2}(\vec{x})$ etc. Note that $\vec{n}_i = (n_{i1}, n_{i2}, n_{i3})$ is the triplet of quantum numbers that completely characterize Hamiltonian's eigenstates. For example, the numeration of the eigenstates could be

$$\vec{n}_1 = (1,1,1)\,,\ \vec{n}_2 = (2,1,1)\,,\ \vec{n}_3 = (1,2,1)\,,\ \text{ etc.} \tag{6.111}$$

with $\vec{n}_1 = (1,1,1)$ being the ground state.

Using the decomposition (6.109) of the thermal density matrix, the mean value can be expressed in the form

$$\left\langle \hat{a}^\dagger_{\vec{n}'_b}\hat{a}^\dagger_{\vec{n}'_c}\hat{a}_{\vec{n}_b}\hat{a}_{\vec{n}_c}\right\rangle_{th} = \sum_{N_{\vec{n}_1},N_{\vec{n}_2},\ldots} P_{\{N_{\vec{n}_i}\}}\,\langle N_{\vec{n}_1}, N_{\vec{n}_2},\ldots|\,\hat{a}^\dagger_{\vec{n}'_b}\hat{a}^\dagger_{\vec{n}'_c}\hat{a}_{\vec{n}_b}\hat{a}_{\vec{n}_c}\,|N_{\vec{n}_1}, N_{\vec{n}_2},\ldots\rangle. \tag{6.112}$$

The only non-zero elements are those with equal number of creation and annihilation operators acting on the same state. The only possible combinations are the following,

$$\begin{aligned}\langle N_{\vec{n}_1}, N_{\vec{n}_2},\ldots|\,\hat{a}^\dagger_{\vec{n}'_b}\hat{a}^\dagger_{\vec{n}'_c}\hat{a}_{\vec{n}_b}\hat{a}_{\vec{n}_c}\,|N_{\vec{n}_1}, N_{\vec{n}_2},\ldots\rangle &= N_{\vec{n}_b}N_{\vec{n}_c}\,\delta_{\vec{n}_c=\vec{n}'_c\neq\vec{n}_b=\vec{n}'_b} + \\ &+ N_{\vec{n}_b}N_{\vec{n}_c}\,\delta_{\vec{n}_c=\vec{n}'_b\neq\vec{n}_b=\vec{n}'_c} + N_{\vec{n}_b}\left(N_{\vec{n}_b}-1\right)\delta_{\vec{n}_c=\vec{n}'_c=\vec{n}_b=\vec{n}'_b},\end{aligned} \tag{6.113}$$

where the "function" $\delta_{\vec{n}_c=\vec{n}'_b\neq\vec{n}_b=\vec{n}'_c}$ equals one when the condition $\vec{n}_c = \vec{n}'_b \neq \vec{n}_b = \vec{n}'_c$ is satisfied and zero when the condition is violated. The final expression for the mean value is,

$$\begin{aligned}\left\langle \hat{a}^\dagger_{\vec{n}'_b}\hat{a}^\dagger_{\vec{n}'_c}\hat{a}_{\vec{n}_b}\hat{a}_{\vec{n}_c}\right\rangle_{th} &= \langle N_{\vec{n}_b}\rangle_{th}\langle N_{\vec{n}_c}\rangle_{th}\delta_{\vec{n}_c=\vec{n}'_c\neq\vec{n}_b=\vec{n}'_b} + \\ &+ \langle N_{\vec{n}_b}\rangle_{th}\langle N_{\vec{n}_c}\rangle_{th}\delta_{\vec{n}_c=\vec{n}'_b\neq\vec{n}_b=\vec{n}'_c} + \left(\left\langle N^2_{\vec{n}_b}\right\rangle_{th} - \langle N_{\vec{n}_b}\rangle_{th}\right)\ \delta_{\vec{n}_c=\vec{n}'_c=\vec{n}_b=\vec{n}'_b}.\end{aligned} \tag{6.114}$$

Substituting, now, back to the expression (6.108) for b_{11} we find

$$\begin{aligned}b_{11} = V_i^2\Bigg[\sum_{\vec{n}}\varphi^2_{\vec{n}}(\vec{x}_{b_1})\,\varphi^2_{\vec{n}}(\vec{x}_{c_1})\cdot\left(\left\langle N^2_{\vec{n}}\right\rangle_{th} - \langle N_{\vec{n}}\rangle_{th}\right) + \sum_{\vec{n}\neq\vec{n}'}\Big(\varphi^2_{\vec{n}'}(\vec{x}_{b_1})\,\varphi^2_{\vec{n}}(\vec{x}_{c_1}) + \\ +\varphi_{\vec{n}}(\vec{x}_{b_1})\,\varphi_{\vec{n}'}(\vec{x}_{c_1})\,\varphi_{\vec{n}'}(\vec{x}_{b_1})\,\varphi_{\vec{n}}(\vec{x}_{c_1})\Big)\cdot\langle N_{\vec{n}}\rangle_{th}\langle N_{\vec{n}'}\rangle_{th}\ \Bigg].\end{aligned} \tag{6.115}$$

Our final corrected expression for the *negativity*, after substituting the expressions (6.59) and (6.115) for I_{bc} and b_{11} respectively, turns out to be

$$\begin{aligned}N\left[\hat{\rho}_{bc}\right] &= \Gamma^4\left(I^2_{bc} - b_{11}\right) \\ &= \Gamma^4 V_i^2\Bigg[\sum_{\vec{n}}\varphi^2_{\vec{n}}(\vec{x}_{b1})\,\varphi^2_{\vec{n}}(\vec{x}_{c1})\left[\langle N_{\vec{n}}\rangle - \left(\left\langle N^2_{\vec{n}}\right\rangle - \langle N_{\vec{n}}\rangle^2\right)\right] - \\ &\qquad - \sum_{\vec{n}\neq\vec{n}'}\varphi^2_{\vec{n}'}(\vec{x}_{b1})\,\varphi^2_{\vec{n}}(\vec{x}_{c1})\,\langle N_{\vec{n}}\rangle\,\langle N_{\vec{n}'}\rangle\Bigg].\end{aligned} \tag{6.116}$$

This formula is utterly surprising! It coincides exactly (minus a positive factor) with the subdeterminant S (5.67) derived using 4^{th}-order continuous variable criteria for the detection of spatial entanglement in the bosonic field. Before we study the behaviour of N, let us make some comments on these findings.

6.5.2 Connection between *Negativity* and Continuous Variable criteria

At this point let's forget about the probes for a while. In Chapter 5 we tried to see whether the bosonic field at finite termperature exhibits non-local particle number correlations, i.e. whether it's spatially entangled. We used 4^{th}-order entanglement criteria for continuous variable systems, and found the following condition (5.67)

$$S = -\left(\sum_a \left(I_a^R\right)^2 \left\langle \hat{N}_a \right\rangle\right) \times \\ \times \left[\sum_k \left(I_k^L\right)^2 \left(I_k^R\right)^2 \left[\left\langle \hat{N}_k \right\rangle - \left(\left\langle \hat{N}_k^2 \right\rangle - \left\langle \hat{N}_k \right\rangle^2\right)\right] - \sum_{k\neq k'} \left(I_k^L\right)^2 \left(I_{k'}^R\right)^2 \left\langle \hat{N}_k \right\rangle \left\langle \hat{N}_{k'} \right\rangle\right],$$

with $I_k^i = \int\limits_L dx\, g\left(x\right) \varphi_k\left(x\right)$. Entanglement exists when $S < 0$ or, equivalently, when the second factor of this expression is positive.

In this chapter we used two quantum probes to locally interact with the field. We calculated their reduced state after the interaction, applied the PPT criterion and found the *negativity* (6.116). The probes get entangled when $N > 0$, a condition which is identical with the second factor of S being positive.

In other words, in both cases entanglement exists when the *same* condition is satisfied,

$$\sum_{\vec{n}} \left(I_{\vec{n}}^L\right)^2 \left(I_{\vec{n}}^R\right)^2 \left[\left\langle \hat{N}_{\vec{n}} \right\rangle - \left(\left\langle \hat{N}_{\vec{n}}^2 \right\rangle - \left\langle \hat{N}_{\vec{n}} \right\rangle^2\right)\right] - \sum_{\vec{n}\neq\vec{n}'} \left(I_{\vec{n}}^L\right)^2 \left(I_{\vec{n}'}^R\right)^2 \left\langle \hat{N}_{\vec{n}} \right\rangle \left\langle \hat{N}_{\vec{n}'} \right\rangle \;\geq\; 0. \tag{6.117}$$

Negativity only seems different because we have done the approximation

$$I_{\vec{n}}^i = \int\limits_{x_{i1}}^{x_{i2}} d^3x\, g\left(\vec{x}\right) \varphi_{\vec{n}}\left(\vec{x}\right) \approx \sqrt{V_i} \varphi_{\vec{n}}\left(\vec{x}_{i1}\right), \quad \text{for } V_i \ll V \tag{6.118}$$

due to the very small probe volume. However we could have derived negativity without using this approximation and the corresponding formula would exactly coincide (6.117), minus a positive factor.

Different approaches gave the same result. The probes get entangled only when we are certain that the field is spatially entangled ($S < 0$), but when $S > 0$ and we're ignorant about field's entanglement the probes do not get entangled. Is (6.117) just a coincidence or is there a deeper meaning in this result? Let us make some speculations, that would be interesting to pursue in future research.

First of all, the 4^{th}-order criterion that we used is just one of the many that can be derived from [84], so were lucky to choose this specific one and achieve the correspondence. A first question is whether the criterion S unveils all the entanglement that general 4^{th}-order criteria can detect. If that's the case, we may conclude that the probes, being correlated with the field's moments up to 4^{th}-order, get entangled only when the field exhibits non-local correlations up to that order. The next step would be to prove this

for a general n-order coupling and criteria. Proving this conjecture would lead us to the following interpretation of continuous variable criteria for non-Gaussian states:

Plausible interpretation

When all possible entanglement criteria of order n (i.e. containing field's moments up to n-order), applied to a field, fail to be violated it will mean that no entanglement can be extracted from that field using 2-level systems coupled to the field's moments up to n-order. Vice versa, if the criteria are *violated then entanglement can be extracted.*
(Note that you can substitute the field with an arbitrary continuous variable system)

We can restrict the order of moments the probes are coupled to via short interaction times, using perturbation theory on the evolution operator. For example in the problem worked out in this chapter, the expansion up to 4^{th}-order in interaction time resulted in a coupling of the probes to moments of the field up to 4^{th}-order as well. Of course, in the case of a finite (and not small) interaction time -when perturbation theory is not applicable- all the field's moments, infinite in number, will get involved. So, if there are any non-local correlations (entanglement) in the field in some arbitrary order of moments n (e.g. even for $n \to \infty$), a finite interaction time with the probes will probably unveil it.

6.5.3 The behaviour of $N\left[\hat{\rho}_{bc}\left(\delta t\right)\right]$ with temperature and separation distance

Now that we have computed the corrected formula for the negativity, we are ready see how the entanglement between the probes behaves under the variation of the field's temperature and separation distance of the probes. Note that all our conclusions about the existence of entanglement between the probes will also hold for the spatial entanglement of the field due to the equivalence found in the previous section. In the Appendix B we have proved the following formulas for the grand-canonical ensemble,

$$\langle N_{\vec{n}} \rangle = \frac{1}{e^{\beta(E_{\vec{n}}-\mu)}-1} \tag{6.119}$$

and

$$\begin{aligned} \left\langle N_{\vec{n}}^2 \right\rangle &= \frac{e^{\beta(E_{\vec{n}}-\mu)}\left(e^{\beta(E_{\vec{n}}-\mu)}+1\right)}{\left(e^{\beta(E_{\vec{n}}-\mu)}-1\right)^2} \\ &= \langle N_{\vec{n}} \rangle^2 \left(\frac{1}{\langle N_{\vec{n}} \rangle}+1\right)\left(\frac{1}{\langle N_{\vec{n}} \rangle}+2\right) \\ &= 2\langle N_{\vec{n}} \rangle^2 + 3\langle N_{\vec{n}} \rangle + 1. \end{aligned} \tag{6.120}$$

It's immediately obvious by using these expressions that

$$\langle N_{\vec{n}} \rangle - \left(\left\langle N_{\vec{n}}^2 \right\rangle - \langle N_{\vec{n}} \rangle^2\right) = -(\langle N_{\vec{n}} \rangle + 1)^2 < 0, \tag{6.121}$$

which means that the *negativity* (6.116) is always negative for every temperature and separation distance of the probes, meaning that entanglement is absent.

Initially we searched for a connection between the amount of entanglement and the critical temperature, since such a connection has been reported elsewhere [94]. However it turned out that the negativity (6.116) is (highly) negative for every temperature $T > 0$, even when $T \to 0$! Initially, this seems to be a very strange result since we would expect that in the absolute zero -where all the bosons occupy the ground state - there would be entanglement. This expectation is based on the following argument; Let's assume that the bosonic gas is not in a thermal state but in a pure state, where all the N bosons are occupy the ground state, i.e.

$$\hat{\rho}_0 = |N, 0, 0, \ldots\rangle \langle N, 0, 0, \ldots| \,. \tag{6.122}$$

Note that this choice is compatible with all the formalism developed in the previous sections, so the formula (6.116) of the negativity still holds for this pure state as well. The negativity now reads

$$N\left[\hat{\rho}_{bc}\right] = \Gamma^4 V_i^2 \, \varphi_{(1,1,1)}\left(\vec{x}_{b1}\right) \varphi_{(1,1,1)}\left(\vec{x}_{c1}\right) N > 0, \tag{6.123}$$

which is non-zero and in contrast to the results given above by the thermal state. The discrepancy lies in the fact that the thermal state, in the grand canonical ensemble, in the limit $T \to 0$, is not equivalent to (6.122). It's straightforward to see why, since the pure state $\hat{\rho}_0$ gives

$$\left\langle N^2_{(1,1,1)} \right\rangle_{\hat{\rho}_0} = \left\langle N_{(1,1,1)} \right\rangle^2_{\hat{\rho}_0} = N^2, \tag{6.124}$$

while the grand canonical ensemble,

$$\left\langle N^2_{(1,1,1)} \right\rangle_{th} \approx 2 \left\langle N_{(1,1,1)} \right\rangle^2_{th} = 2N^2, \tag{6.125}$$

as easily seen by (6.120) for $\left\langle N_{(1,1,1)} \right\rangle \gg 1$. Eq. (6.125) is mainly responsible for the non-appearance of entanglement even near absolute zero $T = 0K$. This kind of behaviour of the grand canonical ensemble for temperatures under the critical is well known in the literature ([102], p. 25). More specifically, the fluctuations of the number of atoms in the condensate becomes huge,

$$\left\langle N^2_{(1,1,1)} \right\rangle - \left\langle N_{(1,1,1)} \right\rangle^2 = \left\langle N_{\vec{n}} \right\rangle^2 + 3 \left\langle N_{\vec{n}} \right\rangle + 1 \gg 1, \tag{6.126}$$

when $\left\langle N_{(1,1,1)} \right\rangle \gg 1$. This represents a pathological feature of the grand canonical ensemble which is due to the fact that we have superposition of states of different total particle number and can be eliminated if we employ, for example, the canonical ensemble. In the latter case the total number of bosons doesn't fluctuate, and only thermal fluctuations are present which vanish for $T \to 0$ as expected [98].

Before continuing our analysis, let us make some comments. It may seem confusing that we get so different results for the different ensembles. What happens in a realistic system in the laboratory? Well, in a realistic system our bosons are massive atoms such as ^4He, ^{87}Rb, and atoms cannot be singly created or destroyed. A strong superselection rule forbids the occurrence in nature of superposition of states with different total number of atoms of a given species. So the behaviour of an experimental system follows the canonical ensemble and not the grand canonical. The reason why the grand canonical ensemble is so

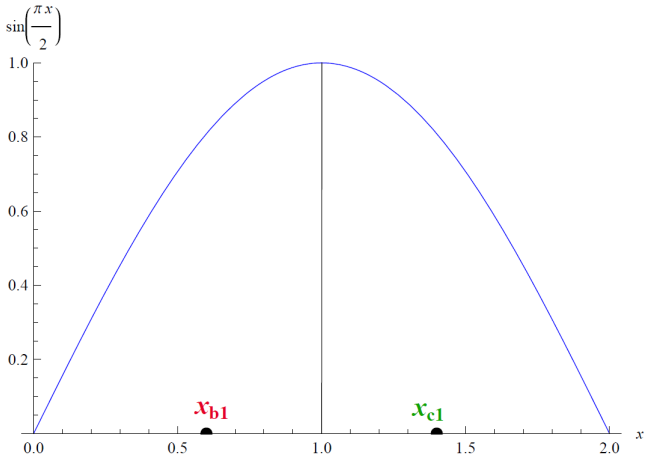

Figure 6.2: The ground state $\varphi_{(n=1)}(x)$ of the bosons is shown, in the case of one dimension and length scale $L = 2$. The middle of the well is depicted at $x = 1$ while the points x_{b1}, x_{c1} approximately represent the position of the two quantum probes.

frequently used, is the great simplification it achieves by making the number of particles in each one-particle state independent with each other through the relaxation of total particle number conservation to *mean* total particle number conservation. Moreover, when N is sufficiently large these two ensembles has been shown to be identical [99] but still some pathologies, like the one we just faced, remain. As a final comment on this issue let us say that the introduction of two-body interactions in the grand canonical ensemble eliminates all its pathologies giving the same results as the canonical distribution [100]. This fact makes the grand canonical ensemble the most convenient for theoretical calculations.

Now lets return to the analysis of the negativity, and specifically to the case where all the bosons are in the ground state and described by the pure state (6.122). At the absolute zero, the two quantum probes get entangled and the amount of their entanglement is given by (6.123),

$$N\left[\hat{\rho}_{bc}\right] = \Gamma^4 V_i^2 \, \varphi_{(1,1,1)}\left(\vec{x}_{b1}\right) \varphi_{(1,1,1)}\left(\vec{x}_{c1}\right) N \geq 0 \quad \text{for} \quad T = 0 \; K.$$

The ground state $\varphi_{(1,1,1)}(\vec{x})$ is depicted in Fig. 6.2 in one spatial dimension. As we see the wavefunction is maximum at the center of the 1D well, so in the 3D case the maximum will be near the center of the cube. If the quantum probes get near that area, where $\varphi_{(1,1,1)}(\vec{x}) \approx 1$, the entanglement gets its maximum value,

$$N_{\max}\left[\hat{\rho}_{bc}\right] = \Gamma^4 V_i^2 N. \tag{6.127}$$

On the other hand, if one of the probes -or both- approach the walls of the trap then $\varphi_{(1,1,1)}\left(\vec{x}_{i1}\right) \to 0$ and negativity vanishes. In other words, the entanglement increases when the both the probes are near the center of the cube and vanishes when at least one of them approaches the walls of the cube.

But what happens for temperatures $T \leq T_C$? As we saw, the grand canonical ensemble gives large fluctuations of the ground state's occupation number and these non-physical fluctuations are responsible for the non-existence of entanglement. It would be interesting

to see what the canonical ensemble would give in this case. However, the calculations in the canonical ensemble -even numerically- are very demanding. The reason is that we have to calculate mean values of the form

$$\langle N_{\vec{n}_k} \rangle = \sum_{N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots} \frac{1}{Z} \exp\left(-\frac{1}{k_B T} \sum_i \frac{\hbar^2 \pi^2}{2mL^2} \vec{n}_i^2 N_{\vec{n}_i} \right) N_{\vec{n}_k}, \tag{6.128}$$

with the extra restriction of the exact total particle number conservation, i.e.

$$\sum_i N_{\vec{n}_i} = N, \tag{6.129}$$

making the summations in (6.128) a very difficult task especially if the number N is very large (which it is).

However we can show that entanglement exists for very low temperatures $T \to 0$ and not only in the absolute zero. In the canonical ensemble, the density matrix of the thermal state will be

$$\hat{\rho}_{th}^c = \sum_{N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots} \frac{1}{Z} \exp\left[-\beta \sum_i E_{\vec{n}_i} N_{\vec{n}_i} \right] |N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots\rangle \langle N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots| \tag{6.130}$$

with the restriction $\sum_i N_{\vec{n}_i} = N$, while the index c on the density matrix reminds us that we're working in the canonical ensemble. As the temperature falls close to zero all the particles gather to the ground state, and the only thermal fluctuation that survives, with very small probability, is having one boson in the first excited state (which is triply degenerate). So, approximately, the thermal state close to absolute zero will be

$$\begin{aligned} \hat{\rho}_{th}^c|_{T\to 0} = (1-3\varepsilon) |N,0,0,0\rangle \langle N,0,0,0| + \\ + \varepsilon |N-1,1,0,0\rangle \langle N-1,1,0,0| + \varepsilon |N-1,0,1,0\rangle \langle N-1,0,1,0| + \\ + \varepsilon |N-1,0,0,1\rangle \langle N-1,0,0,1|, \end{aligned} \tag{6.131}$$

where we have denoted $\left|N_{(1,1,1)}, N_{(2,1,1)}, N_{(1,2,1)}, N_{(1,1,2)}\right\rangle$ and considered the rest of the occupation numbers zero. The three degenerate excited states are equiprobable, each with probability $\epsilon \to 0$, since they have the same energy. It's straightforward to see that the negativity of $\hat{\rho}_{bc}$, when the bosonic field is described by (6.131) near absolute zero, is

$$N\left[\hat{\rho}_{bc}\right]|_{T\to 0} = \Gamma^4 V_i^2 (N-\varepsilon) \quad \text{with} \quad \epsilon \to 0. \tag{6.132}$$

In deriving this result we assumed that both the probes are located near the center of the cubic trap, meaning $\varphi_{(1,1,1)}(\vec{x}_{i1}) \to 1$ and $\varphi_{(2,1,1)}(\vec{x}_{i1}) = \varphi_{(1,2,1)}(\vec{x}_{i1}) = \varphi_{(1,1,2)}(\vec{x}_{i1}) \to 0$, and used the fact

$$\left\langle N_{(1,1,1)} \right\rangle^2_{\hat{\rho}_{th}^c|_{T\to 0}} = \left\langle N^2_{(1,1,1)} \right\rangle_{\hat{\rho}_{th}^c|_{T\to 0}} = (N-\varepsilon)^2, \tag{6.133}$$

which is in sharp contrast to (6.125) of the grand-canonical ensemble.

Concluding, we proved that the quantum probes become entangled not only in the absolute zero $T = 0\ K$ but also in the limit $T \to 0\ K$ showing that entanglement decreases

continuously with the increase of temperature. Moreover it's evident that when the probes are near the center of the cubic trap the amount of entanglement decreases with a slight increase of the temperature, i.e.

$$N\left[\hat{\rho}_{bc}\right]|_{T\to 0} < N\left[\hat{\rho}_{bc}\right]|_{T=0}. \tag{6.134}$$

It would be of great interest to, somehow, do the numerical calculations using the canonical ensemble and see at which temperature the entanglement vanishes. The sure thing is that this temperature lies between the absolute zero $T = 0\ K$ and the critical temperature T_c. Above T_c we can trust the grand-canonical ensemble which gives no entanglement.

Concluding, we saw that the quantum phase transition of the bosonic field plays a major role in the extracted entanglement, since during only that phase entanglement can be extracted in the short-interaction time approximation. In the next section we will see that the *concurrence* exhibits exactly the same behaviour as *negativity*.

6.6 Calculation of Concurrence

In this section we will calculate the *concurrence* $C\left[\hat{\rho}_{bc}\left(\delta t\right)\right]$ of the probes' reduced quantum state after the interaction with the bosonic field. We saw, in the previous section, that the 4^{th}-order terms made a contribution to the Negativity and we expect that such a contribution will be evident in the Concurrence as well. So, in the following calculations we will use the reduced quantum state up to 4^{th} order, i.e.

$$\hat{\rho}_{bc}\left(\delta t\right) = \begin{pmatrix} \Gamma^4 b_{11} & 0 & 0 & 0 \\ 0 & \Gamma^2 I_{bb} & \Gamma^2 I_{bc} & 0 \\ 0 & \Gamma^2 I_{bc} & \Gamma^2 I_{cc} & 0 \\ 0 & 0 & 0 & 1-\Gamma^2\left(I_{bb}+I_{cc}\right) \end{pmatrix}. \tag{6.135}$$

Let us repeat the relevant formulas,

$$C\left(\hat{\rho}_{bc}\right) = \max\left\{0, \sqrt{R_1} - \sqrt{R_2} - \sqrt{R_3} - \sqrt{R_4}\right\}$$

$$R = \hat{\rho}_{bc}\sigma_y \otimes \sigma_y \hat{\rho}^*_{bc} \sigma_y \otimes \sigma_y$$

where R_1, R_2, R_3, R_4 are the decreasingly ordered eigenvalues of the matrix R and σ_y is the second Pauli matrix which has the matrix form

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{6.136}$$

in the representation (6.79) used. It's straightforward to see that $\sigma_y \otimes \sigma_y = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ and matrix R gets the form

$$R = \begin{pmatrix} b_{11}\Gamma^4 & 0 & 0 & 0 \\ 0 & \left(I_{bc}^2 + I_{bb}I_{cc}\right)\Gamma^2 & 2I_{bb}I_{bc}\Gamma^2 & 0 \\ 0 & 2I_{cc}I_{bc}\Gamma^2 & \left(I_{bc}^2 + I_{bb}I_{cc}\right)\Gamma^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{6.137}$$

Next we find the four square-rooted eigenvalues of R to be

$$\begin{gathered}\left(|I_{bc}|+\sqrt{I_{bb}I_{cc}}\right)\Gamma^2,\quad \left||I_{bc}|-\sqrt{I_{bb}I_{cc}}\right|\Gamma^2,\\ \sqrt{b_{11}}\Gamma^2,\quad \sqrt{b_{11}}\Gamma^2.\end{gathered} \tag{6.138}$$

In order to form the formula of concurrence, we are interested in knowing which eigenvalue is the largest since it will take the place of the positive $\sqrt{R_1}$ in the formula. We distinguish two cases:

Case (I): $|I_{bc}|+\sqrt{I_{bb}I_{cc}}>\sqrt{b_{11}}$

In this scenario $\sqrt{R_1}=\left(|I_{bc}|+\sqrt{I_{bb}I_{cc}}\right)\Gamma^2$ is the largest eigenvalue and the concurrence reads

$$C_I\left[\hat{\rho}_{bc}\right]=\left[|I_{bc}|+\sqrt{I_{bb}I_{cc}}-\left||I_{bc}|-\sqrt{I_{bb}I_{cc}}\right|-2\sqrt{b_{11}}\right]\Gamma^2 \tag{6.139}$$

Next we need to consider two sub-cases,

$$\textbf{(I}_a\textbf{)}\quad |I_{bc}|\leq\sqrt{I_{bb}I_{cc}}\quad\text{leads to}\quad C_{I_a}\left[\hat{\rho}_{bc}\right]=2\Gamma^2\left(|I_{bc}|-\sqrt{b_{11}}\right) \tag{6.140}$$

$$\textbf{(I}_b\textbf{)}\quad |I_{bc}|\geq\sqrt{I_{bb}I_{cc}}\quad\text{leads to}\quad C_{I_b}\left[\hat{\rho}_{bc}\right]=2\Gamma^2\left(\sqrt{I_{bb}I_{cc}}-\sqrt{b_{11}}\right). \tag{6.141}$$

Notice that in the case (I_a) entanglement exists only for $|I_{bc}|>\sqrt{b_{11}}$ which exactly agrees with negativity (6.116). This is always true if the two probes are positioned in such places that the one-particle Hamiltonian's eigenfunctions have the same value for both probes, i.e. $\varphi_{\vec{n}}\left(\vec{x}_{b1}\right)=\varphi_{\vec{n}}\left(\vec{x}_{c1}\right)$. For example, in section 6.5.3 we considered both the probes to be very close the center of the cubic trap in order to find the maximum entanglement at the near the absolute zero. In this case it is indeed true, and the two entanglement measures agree completely.

Case (II): $|I_{bc}|+\sqrt{I_{bb}I_{cc}}<\sqrt{b_{11}}$

In this second scenario $\sqrt{R_1}=\sqrt{b_{11}}$ is the largest eigenvalue but since

$$\begin{aligned}\sqrt{R_1}-\sqrt{R_2}-\sqrt{R_3}-\sqrt{R_4}&=\\ &=\sqrt{b_{11}}-\sqrt{b_{11}}-\left(|I_{bc}|+\sqrt{I_{bb}I_{cc}}\right)-\left||I_{bc}|-\sqrt{I_{bb}I_{cc}}\right|\\ &=-\left(|I_{bc}|+\sqrt{I_{bb}I_{cc}}+\left||I_{bc}|-\sqrt{I_{bb}I_{cc}}\right|\right)\\ &\leq 0,\end{aligned} \tag{6.142}$$

the value of concurrence is zero

$$\begin{aligned}C_{II}\left[\hat{\rho}_{bc}\right]&=\max\left\{0,\ \sqrt{R_1}-\sqrt{R_2}-\sqrt{R_3}-\sqrt{R_4}\leq 0\right\}\\ &=0.\end{aligned} \tag{6.143}$$

Once more this agrees exactly with the negativity since entanglement vanishes for

$$|I_{bc}|+\sqrt{I_{bb}I_{cc}}<\sqrt{b_{11}}\quad\Rightarrow\quad|I_{bc}|<\sqrt{b_{11}}. \tag{6.144}$$

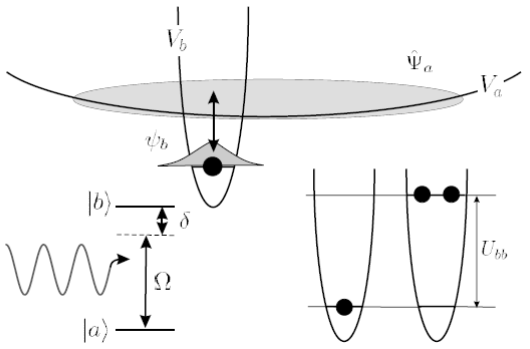

Figure 6.3: *Top*: An AQD is formed, by a tightly confining potential V_b with a localized atom in state b, inside a BEC of atoms in state a, described by $\hat{\psi}_a$, confined by a shallow trap $V_a(\mathbf{x})$. *Bottom*: Atoms in states a and b are coupled by a Raman transition with effective Rabi frequency Ω. A large on-site interaction $U_{bb} > 0$ allows only a single atom inside the AQD. From Recati *et. al.* [104].

Concluding, we have shown the equivalence of the two entanglement measures. All the results we obtained for negativity hold for the concurrence as well, so we refer the reader to Section 6.5.3 for all the results on the existence of entanglement. As a final note let us comment on the fact that the concurrence is of order of magnitude Γ^2 in contrast to the Γ^4 of negativity. Is there a contradiction here? No, there is no contradiction. The answer lies to the fact that concurrence is not an entanglement measure by itself. The real entanglement measure, from which concurrence acquires its meaning as a measure, is the *Entanglement of Formation* (6.137). E_F depends not on $C(\hat{\rho}_{bc})$ but on $\sqrt{1-C(\hat{\rho}_{bc})^2}$ which, indeed, is of order Γ^4.

6.7 Experimental realization of the model Hamiltonian

In this section, we will briefly report on a possible implementation of the interaction Hamiltonian (6.8) between the probes and the bosonic field. Recently, *Recati et. al.* [104] proposed a scheme where Atomic Quantum Dots (AQDs) were coupled to a reservoir of a superfluid Bose-Einstein Condensate.

An AQD is a single atom in a tight trap (see [105]-[107]). This tight 3-dimensional trap is created inside an atomic BEC via focused superimposed laser beams[108], while the condensate is held together by an external potential. The situation is depicted is depicted in Figure 6.3. Atoms in the condensate are in a state with negligible dipole moment, hence cannot interact with the laser-induced trap of the AQD. In order to confine an atom inside the trap, we excite it with a laser (Raman transition) so that it acquires a large dipole moment. Rydberg atoms are well-known for this feature. Once the atomic transition is complete, the atom -which previously belonged to the condensate- strongly interacts with the laser fields that form the AQD and is immediately trapped inside V_b, described now by the confined quantum state ψ_b. Atoms loaded in the AQD repel due to collisional interactions, and in the limit of strong repulsion -achieved via Feshbach resonances [109]-

only one or no atom occupies the AQD while higher occupations are strongly suppressed. This mechanism makes essentially the AQD a *qubit* with pseudo-spin $\frac{1}{2}$. The state $|0\rangle$ represent the AQD when no atoms occupy the confining trap V_b, while $|1\rangle$ represent the AQD with just one atom inside. When an atom of the reservoir (BEC) is confined in the AQD, the total number of atoms in the AQD increases +1 while the total number of atoms in the reservoir decreases -1. In this way our desired interacting term (6.7) is formed, representing a coupling between the BEC and the lowset vibrational state in the AQD via a Raman transition, while spontaneous emission is suppressed by a large detuning from the excited electronic states. This coupling between the reservoir and the AQD, via a Raman transition, is described in the language of second-quantization by the interaction Hamiltonian (6.8) we used.

6.8 Conclusions

In this chapter we studied an entanglement extraction scheme out of a Bose-Einstein Condensate. We did that for two reasons; One of them was to present an alternative way of creating entangled qubits that are usefull to quantum information processing. Our main aim however, coming to the second reason for this study, was to indirectly find out about the entanglement properties of the bosonic field via the observation of the entanglement properties of the probes. In order to solve the problem we worked perturbatively for small interaction times between the probes and the bosonic field. This immediately implies that some information about the field's entanglement, encrypted in higher orders of the perturbative expansion, are lost and our probes were not able to extract that lost entanglement. Whatever entanglement we found, came directly from the field's moments up to 4^{th}-order, i.e. only mean values up to $\left\langle \hat{\psi}_a^{(\dagger)}(x_1)\,\hat{\psi}_a^{(\dagger)}(x_2)\,\hat{\psi}_a^{(\dagger)}(x_3)\,\hat{\psi}_a^{(\dagger)}(x_4)\right\rangle$ are involved, while covariances involving more than four field operators do not contribute. This is an important note, because the non-entanglement of the qubits for some temperatures doesn't necessarily imply that the field is separable at that temperature. In a non-perturbative treatment, corresponding to a finite interaction time, all the field's moments are involved and entanglement could be unveiled for temperatures that our method wasn't able to detect.

We calculated two well-known entanglement measures for the reduced quantum state of the probes after the interaction, the *negativity* and *concurrence*. They both showed almost identical results on the existence of entanglement between the probes. We found entanglement for temperatures near the absolute zero below the critical temperature of the field, while for temperatures above the critical no entanglement was extracted. The exact temperature that signals the onset of entanglement as $T \to 0\ K$ is shown to be in the interval $(0, T_c)$. The maximum entanglement was found in the absolute zero $T = 0\ K$ and decreased with the increase of temperature. Regarding the separation distance between the probes, the maximum entanglement near $T = 0\ K$ was found when both the probes were close to the center of our cubic trap and rapidly decreased to zero if just one of the probes (or both) approached the walls of the trap. That behaviour directly reflected the fact that, the one-particle wavefunction of the field's bosons had maximum amplitude (for $T = 0\ K$) near the center and zero amplitude near the walls ($\forall\ T$).

Moreover, we found a surprising match between the aforementioned entanglement cri-

teria used on the probes, and the 4^{th}-order continuous variable entanglement criterion, of Chapter 5, used on the field. A possible interpretation of this result could be that, all the spatial entanglement of the bosonic field, present in correlations of the field operators up to 4^{th}-order, was unveiled by the probes. However, in order to arrive to a definite conclusion about the validity of such an interpretation, we should calculate all possible continuous-variable criteria up to that order and make sure that they don't unveil entanglement for a wider range of temperatures than the one we used in this project.

Finally, we presented a way of a possible implementation of the local interaction Hamiltonian we used between the probes and the field, showing that such an interaction is experimentally and physically feasible.

Appendix A

On (Partial) Transposition

In this appendix, we will prove various properties of the (partially) transposed density matrix, which is frequently used in deriving entanglement criteria.

The transposition of a density matrix $\hat{\rho}$ is defined by,

$$\langle n|\,\hat{\rho}^T\,|m\rangle = \langle m|\,\hat{\rho}\,|n\rangle\,, \tag{A.1}$$

for a given basis $\{|n\rangle\}$, while the partial transposition in the case of a bipartite system is defined by,

$$\langle nm|\,\hat{\rho}^{PT}\,|kl\rangle = \langle nl|\,\hat{\rho}\,|km\rangle\,, \tag{A.2}$$

where we chose to transpose the second subsystem.

PROPERTIES

[P1] ***The transposed density matrix is a legitimate density matrix***

This is true since the transposition operator preserves the properties,

$$Tr\hat{\rho}^T = Tr\hat{\rho} = 1 \quad \text{and} \quad Tr\big(\hat{\rho}^T\big)^2 = Tr\hat{\rho}^2 < 1. \tag{A.3}$$

The proof is easy. We assume that the transposition is defined with respect to some basis $\{|m\rangle\}$, which we use to dismiss the transposition,

$$Tr\hat{\rho}^T = \sum_m \langle m|\hat{\rho}^T\,|m\rangle = \sum_m \langle m|\hat{\rho}\,|m\rangle = Tr\hat{\rho} = 1, \tag{A.4}$$

$$Tr\big(\hat{\rho}^T\big)^2 = \sum_m \langle m|\big(\hat{\rho}^T\big)^2\,|m\rangle = \sum_m \langle m|(\hat{\rho}\,\hat{\rho})^T\,|m\rangle = \sum_m \langle m|\hat{\rho}^2\,|m\rangle = Tr\hat{\rho}^2 < 1. \tag{A.5}$$

[P2] ***The partially transposed $\hat{\rho}^{PT}$ of a bipartite separable state $\hat{\rho}$ is itself a legitimate density matrix***

Since, for separable states, it's

$$\hat{\rho}^{PT} = \sum_i p_i \hat{\rho}_{i1} \otimes \hat{\rho}_{i2}^T,$$

and using the result from [P1] that $\hat{\rho}_{i2}^T$ is legitimate density matrix, we conclude that $\hat{\rho}^{PT}$ is a legitimate density matrix as well.

[P3] ***The partially transposed*** $\hat{\rho}^{PT}$ ***of a bipartite separable state*** $\hat{\rho}$***: (i) preserves the normalization*** $Tr\hat{\rho}^{PT} = 1$, ***(ii) has the same purity with*** $\hat{\rho}$***, i.e.*** $Tr\left(\hat{\rho}^{PT}\right)^2 = Tr\hat{\rho}^2$,***, while (iii) it does not preserve the moments of higher order, i.e.*** $Tr\left(\hat{\rho}^{PT}\right)^{n>2} \neq Tr\hat{\rho}^{n>2}$ ***in general***

Let us prove these properties one at a time.

(i)

$$\begin{aligned} Tr\hat{\rho}^{PT} &= \sum_{n,m} {}_1\langle n| \otimes {}_2\langle m| \left(\sum_i p_i \hat{\rho}_{i1} \otimes \hat{\rho}_{i2}^T \right) |n\rangle_1 \otimes |m\rangle_2 \\ &= \sum_i p_i \sum_n {}_1\langle n| \hat{\rho}_{i1} |n\rangle_1 \sum_m {}_2\langle m| \hat{\rho}_{i2}^T |m\rangle_2 \\ &= \sum_i p_i \underbrace{Tr\hat{\rho}_{i1}}_{=1} \underbrace{Tr\hat{\rho}_{i2}^T}_{=1} = \sum_i p_i \\ &= 1 \end{aligned} \tag{A.6}$$

(ii)

$$\begin{aligned} Tr\left(\hat{\rho}^{PT}\right)^2 &= Tr\left[\left(\sum_i p_i \hat{\rho}_{i1} \otimes \hat{\rho}_{i2}^T \right)^2 \right] = Tr\left[\sum_{i,j} p_i p_j \hat{\rho}_{i1} \hat{\rho}_{j1} \otimes \hat{\rho}_{i2}^T \hat{\rho}_{j2}^T \right] \\ &= \sum_{i,j} p_i p_j Tr_1\left(\hat{\rho}_{i1}\hat{\rho}_{j1}\right) \sum_m {}_2\langle m| \left(\hat{\rho}_{j2}\hat{\rho}_{i2}\right)^T |m\rangle_2 \end{aligned} \tag{A.7}$$

At this point we have chosen the appropriate basis $\{|m\rangle_2\}$, in the Hilbert space H_2, with respect to which the action of the transposition operation has been defined, so the transposition can be dismissed.

$$\begin{aligned} &= \sum_{i,j} p_i p_j Tr_1\left(\hat{\rho}_{i1}\hat{\rho}_{j1}\right) Tr_2 \underbrace{\left(\hat{\rho}_{j2}\hat{\rho}_{i2}\right)}_{\text{cyclicperm.}} \\ &= \sum_{i,j} p_i p_j Tr_1\left(\hat{\rho}_{i1}\hat{\rho}_{j1}\right) Tr_2\left(\hat{\rho}_{i2}\hat{\rho}_{j2}\right) \\ &= Tr\left[\sum_{i,j} p_i p_j \, \hat{\rho}_{i1}\hat{\rho}_{j1} \otimes \; \hat{\rho}_{i2}\hat{\rho}_{j2} \right] \\ &= Tr\hat{\rho}^2. \end{aligned} \tag{A.8}$$

(iii) The proof of the in-equality between the higher moments is based on the inability of cyclic permutation, as is possible in the first equality of (A.8). So, up to that point we proceed exactly like in (A.7), but when it comes the point to cyclic permute the operators a problem appears. Let us work, for example, the case $n = 3$,

$$\begin{aligned} \sum_m {}_2\langle m| \hat{\rho}_{i2}^T \hat{\rho}_{j2}^T \hat{\rho}_{k2}^T |m\rangle_2 = \sum_m {}_2\langle m| \left(\hat{\rho}_{k2}\hat{\rho}_{j2}\hat{\rho}_{i2}\right)^T |m\rangle_2 = Tr_2 \underbrace{\left(\hat{\rho}_{k2}\hat{\rho}_{j2}\hat{\rho}_{i2}\right)}_{\text{cyclicperm.}} \\ = Tr_2\left(\hat{\rho}_{i2}\hat{\rho}_{k2}\hat{\rho}_{j2}\right) \\ \neq Tr_2\left(\hat{\rho}_{i2}\hat{\rho}_{j2}\hat{\rho}_{k2}\right), \end{aligned} \tag{A.9}$$

which means, that, $Tr\left(\hat{\rho}^{PT}\right)^3 \neq Tr\hat{\rho}^3$ in general. Same for $n > 3$. We conclude that,

$$Tr\left(\hat{\rho}^{PT}\right)^n \neq Tr\hat{\rho}^n, \tag{A.10}$$

in general.

Some Remarks .

The use of partial transposition on operators can be quite tricky. We emphasized continuously in our previous analysis that transposition is defined with respect to some particular basis. But, why? Say that someone gives you the density matrix $\hat{\rho}^T$ without specifying the basis with respect to which this transposition operation has been defined. Can you know what this state is? The answer is no, for the following reason. Consider two different bases, $\{|a_1\rangle\}, \{|b_2\rangle\}$. The matrix elements of $\hat{\rho}^T$, in these two bases, will be

$$\langle a_1| \hat{\rho}^T \left|a'_1\right\rangle = \left\langle a'_1\right| \hat{\rho} \left|a_1\right\rangle \rightarrow \rho^{(1)}_{a'_1 a_1}, \tag{A.11}$$

$$\langle b_2| \hat{\rho}^T \left|b'_2\right\rangle = \left\langle b'_2\right| \hat{\rho} \left|b_2\right\rangle \rightarrow \rho^{(2)}_{b'_2 b_2}. \tag{A.12}$$

The two matrices $\rho^{(1)}_{a'_1 a_1}, \rho^{(2)}_{b'_2 b_2}$ are not equivalent due to the fact, that, the transposition operation is not a unitary operation (i.e. it's not described by unitary matrix), while equivalent matrices are related by a unitary operations only. So, the density matrix $\hat{\rho}^T$ is not an unambiguously defined state, if we are not told in what basis the transposition operator is supposed to act. At this point, we would like to give an example that demonstrates this in-equivalence.

Example Consider a qubit in the following mixed state,

$$\hat{\rho} = \frac{1}{2} |+, z\rangle \langle +, z| + \frac{1}{2} |+, y\rangle \langle +, y|, \tag{A.13}$$

where $|+, i\rangle$ is the state with spin-up in the i-direction. We know that the two bases $\{|\pm, z\rangle\}, \{|\pm, y\rangle\}$ are related by,

$$|\pm, y\rangle = \frac{1}{\sqrt{2}} \left(|+, z\rangle \pm i |-, z\rangle\right), \tag{A.14}$$

$$|+, z\rangle = \frac{1}{\sqrt{2}} \left(|+, y\rangle + |-, y\rangle\right), \;\; |-, z\rangle = \frac{-i}{\sqrt{2}} \left(|+, y\rangle - |-, y\rangle\right). \tag{A.15}$$

Our goal is to calculate the mean value of the Pauli matrix σ_y, which in the basis $\{|\pm, z\rangle\}$ has the matrix representation $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_z$, while in the basis $\{|\pm, y\rangle\}$ is represented by $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_y$. We will see that if we calculate the mean value $\langle \sigma_y \rangle_{\hat{\rho}}$ with respect to $\hat{\rho}$, the final result will be independent of the basis we used to calculate the mean value. On the other hand, we will also consider $\hat{\rho}^T$ and compute $\langle \sigma_y \rangle_{\hat{\rho}^T}$ with respect to this state as well in two different bases, where the transposition operation will act each time in the basis given. We will find that the different bases give a different mean value, confirming what we said above. The density matrix (A.13) can be represented in the two bases as,

$$\hat{\rho} \rightarrow \frac{1}{4} \begin{pmatrix} 3 & -i \\ i & 1 \end{pmatrix}_z, \; \frac{1}{4} \begin{pmatrix} 3 & 1 \\ 1 & 1 \end{pmatrix}_y, \tag{A.16}$$

where the subscript indicates the basis with respect to which a matrix representation has been formed.

• The mean value $\langle\hat{\sigma}_y\rangle_{\hat{\rho}} = Tr\hat{\rho}\hat{\sigma}_y$ can easily be seen to be independent to the choice of basis,

$$\text{Basis } \{|\pm,z\rangle\}: \quad Tr_z\hat{\rho}\hat{\sigma}_y = Tr\left[\frac{1}{4}\begin{pmatrix} 3 & -i \\ i & 1 \end{pmatrix}_z \cdot \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_z\right] = \frac{1}{4}Tr\begin{pmatrix} 1 & -3i \\ i & 1 \end{pmatrix} = \frac{1}{2} \tag{A.17}$$

$$\text{Basis } \{|\pm,y\rangle\}: \quad Tr_y\hat{\rho}\hat{\sigma}_y = Tr\left[\frac{1}{4}\begin{pmatrix} 3 & 1 \\ 1 & 1 \end{pmatrix}_y \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_y\right] = \frac{1}{4}Tr\begin{pmatrix} 3 & -1 \\ 1 & -1 \end{pmatrix} = \frac{1}{2}. \tag{A.18}$$

The mean values (A.17),(A.18) coincide as expected.

• Let's see what happens with the transposed matrix $\hat{\rho}^T$; do the mean values $Tr_z\hat{\rho}^T\hat{\sigma}_y$, and $Tr_y\hat{\rho}^T\hat{\sigma}_y$ coincide?

$$\text{Basis } \{|\pm,z\rangle\}: \quad \hat{\rho} = \frac{1}{4}\begin{pmatrix} 3 & -i \\ i & 1 \end{pmatrix}_z \rightarrow \quad \hat{\rho}_z^T = \frac{1}{4}\begin{pmatrix} 3 & i \\ -i & 1 \end{pmatrix}_z = \frac{1}{2}|+,z\rangle\langle+,z| + \frac{1}{2}|-,y\rangle\langle-,y| \neq \hat{\rho}$$

$$Tr_z\,\hat{\rho}_z^T\hat{\sigma}_y = Tr_z\left[\frac{1}{4}\begin{pmatrix} 3 & i \\ -i & 1 \end{pmatrix}_z \cdot \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_z\right] = \frac{1}{4}Tr\begin{pmatrix} -1 & -3i \\ i & -1 \end{pmatrix}_z = -\frac{1}{2}. \tag{A.19}$$

$$\text{Basis } \{|\pm,y\rangle\}: \quad \hat{\rho} = \frac{1}{4}\begin{pmatrix} 3 & 1 \\ 1 & 1 \end{pmatrix}_y \rightarrow \quad \hat{\rho}_y^T = \frac{1}{4}\begin{pmatrix} 3 & 1 \\ 1 & 1 \end{pmatrix}_y = \frac{1}{2}|+,z\rangle\langle+,z| + \frac{1}{2}|+,y\rangle\langle+,y| = \hat{\rho}$$

$$Tr_y\,\hat{\rho}_y^T\hat{\sigma}_y = Tr_z\left[\frac{1}{4}\begin{pmatrix} 3 & 1 \\ 1 & 1 \end{pmatrix}_y \cdot \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_y\right] = Tr_y\hat{\rho}\hat{\sigma}_y = \frac{1}{2}. \tag{A.20}$$

It's obvious that the mean values (A.19), (A.20) are different confirming what we initially expected. We repeat that this difference is due to the fact that the transposition of an operator in two different basis gives (in general) two different matrices.

Appendix B

Bose-Einstein Condensation

In this section we will review the Bose-Einstein Condensation (BEC) of a free non-relativistic bosonic field, based on the original paper of London [101]. We will consider N identical bosons to be jointly described by a thermal state at finite temperature, which in the grand-canonical ensemble is given by

$$\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H}-\mu\hat{N})}, \text{ with } Z = Tr\hat{\rho}, \tag{B.1}$$

where $\beta = 1/k_B T$, $\hat{N} = \sum_i \hat{a}^\dagger_{\vec{n}_i} \hat{a}_{\vec{n}_i}$ is the number operator, and the chemical potential μ is determined by the condition that the *mean* number of particles is conserved (i.e. not exact conservation),

$$N = \sum_i \langle \hat{n}_{\vec{n}_i} \rangle = \sum_i \left\langle \hat{a}^\dagger_{\vec{n}_i} \hat{a}_{\vec{n}_i} \right\rangle. \tag{B.2}$$

As is obvious we work in the second quantization formalism (see Sections 3.1 for details), where the annihilation/creation operators $\left\{\hat{a}^\dagger_{\vec{n}_i}, \hat{a}_{\vec{n}_i}\right\}$ lower/raise the number of particles of the one-particle Hamiltonian's eigenstate $|E_{\vec{n}_i}\rangle$, and the components of $\vec{n}_i$ symbolizes the quantum numbers characterizing the state. Moreover, when we say that the number of particles is not exactly conserved (since only the mean value is), we don't mean that "particles are lost/gained". We mean that the quantum state of the gas is in a superposition of states of different particle number. For a discussion on why we use the grand-canonical ensemble, instead of the canonical, see Section 6.5.3. The Hamiltonian of the N free and non-relativistic identical bosons, is

$$\hat{H} = \sum_i E_{\vec{n}_i} \hat{a}^\dagger_{\vec{n}_i} \hat{a}_{\vec{n}_i}, \tag{B.3}$$

so the density matrix becomes

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \sum_i \left(E_{\vec{n}_i} - \mu\right) \hat{n}_{\vec{n}_i}} \tag{B.4}$$

In order to evaluate (B.2), we need to calculate the mean values $\langle \hat{n}_{\vec{n}_i} \rangle$ with respect to the density matrix $\hat{\rho}$. In the calculations below we will take the trace with respect to the eigenstates of definite particle number $|N_{\vec{n}_i}\rangle$ of the commuting operators $\{\hat{n}_{\vec{n}_i}\}$, i.e.

$$\hat{n}_{\vec{n}_i} |N_{\vec{n}_i}\rangle = N_{\vec{n}_i} |N_{\vec{n}_i}\rangle . \tag{B.5}$$

So, the decomposition of unity in Fock space becomes,

$$\hat{1} = \sum_{N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots} |N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots\rangle \otimes \langle N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots| , \tag{B.6}$$

where $|N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots\rangle \equiv |N_{\vec{n}_1}\rangle \otimes |N_{\vec{n}_2}\rangle \otimes \cdots$. Now it's straightforward to evaluate the mean value,

$$\begin{aligned}\langle \hat{n}_{\vec{n}_i}\rangle = Tr\hat{\rho}\ \hat{n}_{\vec{n}_i} &= \sum_{N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots} \langle N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots|\, \hat{\rho}\, \hat{n}_{\vec{n}_i}\, |N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots\rangle \\ &= \sum_{N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots} N_{\vec{n}_i}\, \langle N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots|\, \hat{\rho}\, |N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots\rangle,\end{aligned} \tag{B.7}$$

where

$$\begin{aligned}\langle N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots|\, \hat{\rho}\, |N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots\rangle &= \frac{1}{Z}\ \langle N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots|\, e^{-\beta\sum\limits_j \left(E_{\vec{n}_j}-\mu\right)\ \hat{n}_{\vec{n}_j}}\, |N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots\rangle \\ &= \frac{1}{Z}\ \langle N_{\vec{n}_1}|\, e^{-\beta\left(E_{\vec{n}_1}-\mu\right)\ \hat{n}_{\vec{n}_1}}\, |N_{\vec{n}_1}\rangle \cdot \langle N_{\vec{n}_2}|\, e^{-\beta\left(E_{\vec{n}_2}-\mu\right)\ \hat{n}_{\vec{n}_2}}\, |N_{\vec{n}_2}\rangle\ \cdots \\ &= \frac{e^{-\beta\sum\limits_j \left(E_{\vec{n}_j}-\mu\right)\ N_{\vec{n}_j}}}{\sum\limits_{N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots} e^{-\beta\sum\limits_j \left(E_{\vec{n}_j}-\mu\right)\ N_{\vec{n}_j}}}.\end{aligned} \tag{B.8}$$

Hence, we have

$$\begin{aligned}\langle \hat{n}_{\vec{n}_i}\rangle &= \frac{\sum\limits_{N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots} N_{\vec{n}_i}\ e^{-\beta\sum\limits_j \left(E_{\vec{n}_j}-\mu\right)\ N_{\vec{n}_j}}}{\sum\limits_{N_{\vec{n}_1}, N_{\vec{n}_2}, \ldots} e^{-\beta\sum\limits_j \left(E_{\vec{n}_j}-\mu\right)\ N_{\vec{n}_j}}} = \frac{\sum\limits_{\left\{N_{\vec{n}_k}\right\}\neq N_{\vec{n}_i}} e^{-\beta\sum\limits_{j\neq i} \left(E_{\vec{n}_j}-\mu\right)\ N_{\vec{n}_j}}}{\sum\limits_{\left\{N_{\vec{n}_k}\right\}\neq N_{\vec{n}_i}} e^{-\beta\sum\limits_{j\neq i} \left(E_{\vec{n}_j}-\mu\right)\ N_{\vec{n}_j}}} \cdot \frac{\sum\limits_{N_{\vec{n}_i}} N_{\vec{n}_i}\ e^{-\beta\left(E_{\vec{n}_i}-\mu\right)\ N_{\vec{n}_i}}}{\sum\limits_{N_{\vec{n}_i}} e^{-\beta\left(E_{\vec{n}_i}-\mu\right)\ N_{\vec{n}_i}}} \\ &= \frac{1}{e^{\beta\left(E_{\vec{n}_i}-\mu\right)}-1},\end{aligned} \tag{B.9}$$

where we used the identities

$$\sum_{n=0}^{\infty} e^{a\cdot n} = -\frac{1}{e^a-1}, \quad \sum_{n=0}^{\infty} n\, e^{a\cdot n} = \frac{e^a}{(e^a-1)^2}. \tag{B.10}$$

Before analysing the condensation phenomenon, we would like to do a few more calculations regarding various mean values that are useful in *Part III*. In particular, we would like to calculate $\left\langle \hat{n}_{\vec{n}_i}\, \hat{n}_{\vec{n}_j}\right\rangle\big|_{i\neq j}$ and $\left\langle \hat{n}^2_{\vec{n}_i}\right\rangle$,

$$\begin{aligned}\left\langle \hat{n}_{\vec{n}_i}\, \hat{n}_{\vec{n}_j}\right\rangle\big|_{i\neq j} &= \frac{\sum\limits_{\left\{N_{\vec{n}_k}\right\}\neq N_{\vec{n}_i}, N_{\vec{n}_j}} e^{-\beta\sum\limits_{l\neq i,j} \left(E_{\vec{n}_l}-\mu\right)\ N_{\vec{n}_l}}}{\sum\limits_{\left\{N_{\vec{n}_k}\right\}\neq N_{\vec{n}_i}, N_{\vec{n}_j}} e^{-\beta\sum\limits_{l\neq i,j} \left(E_{\vec{n}_l}-\mu\right)\ N_{\vec{n}_l}}} \cdot \left(\frac{\sum\limits_{N_{\vec{n}_i}} N_{\vec{n}_i}\ e^{-\beta\left(E_{\vec{n}_i}-\mu\right)\ N_{\vec{n}_i}}}{\sum\limits_{N_{\vec{n}_i}} e^{-\beta\left(E_{\vec{n}_i}-\mu\right)\ N_{\vec{n}_i}}}\right) \cdot \left(\frac{\sum\limits_{N_{\vec{n}_j}} N_{\vec{n}_j}\ e^{-\beta\left(E_{\vec{n}_j}-\mu\right)\ N_{\vec{n}_j}}}{\sum\limits_{N_{\vec{n}_j}} e^{-\beta\left(E_{\vec{n}_j}-\mu\right)\ N_{\vec{n}_j}}}\right) \\ &= \frac{1}{e^{\beta\left(E_{\vec{n}_i}-\mu\right)}-1} \cdot \frac{1}{e^{\beta\left(E_{\vec{n}_j}-\mu\right)}-1},\end{aligned} \tag{B.11}$$

where we used the identities (B.10), and similarly

$$\left\langle \hat{n}^2_{\vec{n}_i} \right\rangle = \frac{\sum\limits_{N_{\vec{n}_i}} N^2_{\vec{n}_i}\, e^{-\beta\left(E_{\vec{n}_i}-\mu\right)\, N_{\vec{n}_i}}}{\sum\limits_{N_{\vec{n}_i}} e^{-\beta\left(E_{\vec{n}_i}-\mu\right)\, N_{\vec{n}_i}}} = \frac{e^{\beta\left(E_{\vec{n}_i}-\mu\right)}\left(e^{\beta\left(E_{\vec{n}_i}-\mu\right)}+1\right)}{\left(e^{\beta\left(E_{\vec{n}_i}-\mu\right)}-1\right)^2}, \tag{B.12}$$

where we used another identity,

$$\sum_{n=0}^{\infty} n^2\, e^{a\cdot n} = -\frac{e^a\left(e^a+1\right)}{\left(e^a-1\right)^3}. \tag{B.13}$$

Now, let's continue to examine how a condensation phenomenon can emerge from this system. We substitute $\langle \hat{n}_{\vec{n}_i} \rangle$ in (B.2), and we get the following condition that determines the chemical potential,

$$N = \sum_i \frac{1}{e^{\left(E_{\vec{n}_i}-\mu(T)\right)/k_B T}-1}, \tag{B.14}$$

where we have made the dependence on the temperature explicit, $\mu = \mu\,(\mathrm{T})$ for given N. The quantity μ has to depend on the temperature, since all the other parameters are fixed, and something has to account for variations of temperature. At this point, notice that there could be a degeneration where various states with different quantum numbers $\vec{n}_i$ correspond to the same energy. If this is true, together with all the details, it solely depends on the particular Hamiltonian. We re-express (B.14) in an equivalent form, with all the degenerate states gathered together,

$$N = \sum_{i=0}^{\infty} \frac{g_i}{e^{(E_i-\mu(T))/k_B T}-1}, \tag{B.15}$$

where the different E_i are *different* energy levels and g_i is the number of states with the same energy E_i. For $i = 0$, we get the ground state E_0 which could be set to be zero but that's not necessary so let's not make such an assumption.

What is the range of possible values for $\mu(T)$? For a given temperature, the number of particles with energy E_0, i.e. they occupy all those degenerate states with the same energy E_0, is (for $i = 0$)

$$N_0 = \frac{1}{e^{(E_0-\mu(T))/k_B T}-1}. \tag{B.16}$$

Since a particle number, like N_0, should always be a non-negative number we require that

$$N_0 \geq 0 \quad \Rightarrow \quad \mu\,(T) < E_0, \ \ \forall T, \tag{B.17}$$

where we have excluded the possibility that $\mu(T) = E_0$ since N_0 will become infinite when, at the same time, there isn't an infinite mean number of particles in the gas. It's also straightforward to see from (B.15)that by increasing the temperature, $\mu(T)$ is decreasing, while if the temperature is decreasing then $\mu(T)$ is increasing, in order for the total mean number of particles to be conserved, i.e.

$$\begin{aligned} T \ \uparrow \ &\Rightarrow \quad \mu\,(T) \ \downarrow \\ T \ \downarrow \ &\Rightarrow \quad \mu\,(T) \ \uparrow . \end{aligned} \tag{B.18}$$

We will explore the existence of a critical temperature T_C that signals a condensation phenomenon, and we do that using physical arguments, without using the usual derivation that converts sums into integrals etc. For the latter, one shall study the literature [101], [102], [103].

Let's acknowledge the fact, that the ground state is only one state (or a few), while the excited states are vast in number, so there Let us ask the following question; If we disregard the number of particles in the ground state, and look only at the total number of particles in all the excited states, can this number account for all the particles N for every temperature? Or the ground state is necessary in the description? Since we consider N to be very large ($N \to \infty$), the latter statement means that the ground state is macroscopically occupied by a vast number of particles. Let's see, by hypothesizing that it is possible for the excited states to account for all the particles, i.e.

$$N = \sum_{i \neq 0} N_i = \sum_{i \neq 0} \frac{g_i}{e^{(E_i - \mu(T))/k_B T} - 1}. \tag{B.19}$$

Now, start lowering the temperature, $T \downarrow$. As a consequence, the chemical potential will start rising $\mu(T) \uparrow$, as in (B.18). If $\mu(T) \uparrow$ in the equation (B.19) has a solution, then the excited states can indeed account for all the particles N meaning that the number that occupy the ground state is negligible. This is true, until the temperature has been decreased so much that $\mu(T) \uparrow$ approaches its upper bound (B.17),

$$\mu(T) \to E_0 < E_1 \leq \ldots, \tag{B.20}$$

and cannot increase with the same rate as temperature decreases in order to conserve the total number of particles N. So, we witness a *discontinuity* that signals a critical temperature, below which the excited states cannot account for the total number of particles N, meaning that the occupation of the ground state cannot be negligible any more, and since $N \to \infty$, the ground state occupation will be macroscopic ($N_0 \propto N$). So, there is a critical temperature T_C for which,

$$\mu(T_C) \simeq E_0 < E_1, \tag{B.21}$$

and T_C can be computed, by substituting (B.21) in (B.19), as a solution of the following equation,

$$N = \sum_{i \neq 0} \frac{g_i}{e^{(E_i - E_0)/k_B T_C} - 1}. \tag{B.22}$$

Very briefly, this is the way the condensation phenomenon appears in the grand-canonical ensemble formalism. Below a particular critical temperature T_C, the particles start to massively occupy the ground state. The "discontinuity" stems from the fact that for every temperature $T > T_C$ the occupation of the ground state is negligible, while for $T < T_C$ there is a sudden rise in the rate of ground state's occupation. Besides experiment, numerical calculations using the canonical ensemble have shown that the two ensembles totally agree in the prediction of the condensation at finite temperature T_C. Now, regarding the particular value of the temperature T_C, this is totally dependent on the Hamiltonian and in this Appendix will not present any specific example, for that we refer to the aforementioned literature. So, depending on the situation, T_C could range from zero to a finite value.

Bibliography

[1] M. E. Peskin, D. V. Schroeder, *An Introduction to Quantum Field Theory* (Westview Press, 1995)

[2] A. M. Gleason, J. Math. Mech. **6**, 885 (1957)

[3] R. Horodecki, *et. al.*, Rev. Mod. Phys. **81**, 865b•"942 (2009)

[4] O. Guhne, G. Toth, Phys. Rep. **474**, 1 (2009)

[5] M. A. Nielsen, I. L. Chuang, *Quantum computation and quantum information* (Cambridge University Press, 2010)

[6] E. Desurvire, *Classical and Quantum Information Theory: An introduction for the Telecom Scientist* (Cambridge University Press, 2009)

[7] J. Preskill, *Lecture notes on Quantum information and computation* (Caltech, 1997)

[8] A. Peres , *Quantum Theory: Concepts and Methods* (Kluwer Academic Publishers, 2002)

[9] A. Einstein, B. Podolsky and N. Rosen, Phys. Rev. **47**, 777 (1935)

[10] M. Schlosshauer, Rev. Mod. Phys. **76**, 1267-1305 (2005)

[11] J. Bell, Physics, **1**, 195 (1964)

[12] J. F. Clauser, M. A. Horne, A. Shimony and R. A. Holt, Phys. Rev. Lett. **23**, 880 (1969)

[13] A. Peres, Am. J. Phys., **46**, 7 (1978)

[14] S. J. Freedman and J. F. Clauser, Phys. Rev. Lett. **28**, 938b•"941 (1972)

[15] A. Aspect, J. Dalibard and G. Roger, Phys. Rev. Lett. **49**, 25 (1982)

[16] S. Vongehr, arXiv:1207.5294v3 (2012)

[17] G. Weihs, *et. al.*, Phys. Rev. Lett. **81**, 5039b•"5043 (1998)

[18] M. A. Rowe *et. al.*, Nature **409**, 791-794 (2001)

[19] M. Ansmann *et. al.*, Nature **461**, 504-506 (2009)

[20] E. Santos, arXiv:quant-ph/0410193v1 (2004)

[21] B. S. Cirel'son, Lett. Math. Phys. **4** 93 (1980)

[22] S. Popescu and D. Rohrlich, Found. Phys. **24** 379 (1994)

[23] A. Peres, Found. Phys. **1**, 11 (1984)

[24] T. Isobe and S. Tanimura, Prog. Theor. Phys. **124** 191 (2010)

[25] N. Gisin, Phys. Lett. A **154** 201 (1991)

[26] R. F. Werner, Phys. Rev. A **40** 8 (1989)

[27] Cao Hai-Jing *et. al.* Chin. Phys. Soc. **15** 5 (2006)

[28] S. Popescu, Phys. Rev. Lett. **72** 6 (1994)

[29] C. H. Bennett and S. J. Wiesner, Phys. Rev. Lett. **69**, 2881 (1992)

[30] N. Gisin *et. al.*, Rev. Mod. Phys. **74**, 145 (2002)

[31] P. W. Shor, SIAM Rev. **41**, 303 (1999)

[32] L. A. Lugiato *et. al.*, J. Opt. B: Quantum Semiclass. Opt. **4**, S176 (2002)

[33] L. Amico *et. al.*, Rev. Mod. Phys. **80**, 517b•“576 (2008)

[34] L.-A. Wu, M. S. Sarandy, and D. A. Lidar, Phys. Rev. Lett. **93**, 250404 (2004)

[35] Shi-Jian Gu *et. al.* Phys. Rev. Lett. **93**, 8 (2004)

[36] C. Brukner, V. Vedral and A. Zeilinger, Phys. Rev. A **73**, 012110 (2006)

[37] V. Vedral, New J. Phys. **6**, 102 (2004)

[38] I. Fuentes *et. al.*, Phys. Rev. D **82**, 045030 (2010)

[39] D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998)

[40] D. Bacon *et. al.*, Phys. Rev. Lett. **85**, 1758 (2000)

[41] P. Zanardi *et. al.*, Phys. Rev. Lett. **92**, 060402 (2004)

[42] N. L. Harshman and K. S. Ranade, Phys. Rev. A **84**, 012303 (2011)

[43] W. Thirring *et. al.*, Eur. Phys. J. D **64**, 181 (2011)

[44] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996)

[45] M. Horodecki *et. al.*, Phys. Rev. A **223**, 1 (1996)

[46] O. Rudolph, Phys. Rev. A **67**, 032312 (2003)

[47] K. Chen, L.-A. Wu and L. Yang, Quantum Inf. Comp. **3**, 193 (2003)

[48] B. Terhal, Phys. Lett. A **271**, 319 (2000)

[49] M. Lewenstein *et. al.*, Phys. Rev. A **62**, 052310 (2000)

[50] M. Lewenstein *et. al.*, Phys. Rev. A **63**, 044304 (2001)

[51] C. H. Bennett *et. al.* Phys. Rev. A **53**, 2046b•“2052 (1996)

[52] C. H. Bennett *et. al.* Phys. Rev. Lett. **76**, 5 (1996)

[53] M. Horodecki *et. al.*, Phys. Rev. Lett. **78**, 4 (1997)

[54] M. Horodecki *et. al.*, Phys. Rev. Lett. **80**, 24 (1998)

[55] P. Horodecki, Phys. Lett. A **232**, 333 (1997)

[56] L. Clarisse, *Entanglement Distillation: A Discourse on Bound Entanglement in Quantum Information Theory*, Ph.D. thesis, University of York, arXiv:quant-ph/0612072v1 (2006)

[57] C. H. Bennett *et. al.* Phys. Rev. Lett. **78**, 2031 (1996)

[58] C. H. Bennett *et. al.* Phys. Rev. A **54**, 3824 (1996)

[59] V. Vedral *et. al.* Phys. Rev. Lett. **78**, 2275 (1997)

[60] M. B. Plenio and S. Virmani, Quantum Inf. Comp. **7**, 1 (2006), eprint arXiv:quant-ph/0504163

[61] V. Coffman, J. Kundu and W. K. Wootters, Phys. Rev. A **61**, 052306 (2000)

[62] P. Kok and B. W. Lovett, *Introduction to Optical Quantum Information Processing* (Cambridge University Press, 2010)

[63] S. L. Braunstein and P. van Loock, Rev. Mod. Phys. **77**, 513 (2005)

[64] G. Adesso and F. Illuminati, J. Phys. A: Math. Theor. **40**, 7821b•"7880 (2007)

[65] G. Adesso, *Entanglement of Gaussian States*, Ph.D. thesis, University of Salerno (2007), url: https://www.maths.nottingham.ac.uk/personal/ga/papers/Adesso_PhD.pdf

[66] E. Wigner, Physical Review **40**, 749 (1932)

[67] M. Hillery, R. F. O' Connell, M. O. Scully and E. P. Wigner, Physical Reports **106**, 121 (1984)

[68] R. L. Hudson, Reports on Mathematical Physics **6**, 249 (1974)

[69] R. R. Puri, *Mathematical Methods of Quantum Optics* (Springer-Berlin, 2011)

[70] S. Olivares, *Quantum optics in the phase space - A tutorial on Gaussian states*, eprint arXiv:quant-ph/1111.0786v2

[71] E. Schrodinger, Sitzungsber. Preuss. Akad. Wiss. p. 296 (Berlin, 1930); H. P. Robertson, Phys. Rev. **35** 667A (1930); **46** 794 (1934)

[72] V. V. Dodonov, E. V. Kurmyshev and V. I. Man'ko, Phys. Lett. **79A**, 2,3 (1980)

[73] R. Simon, N. Mukunda and B. Dutta, Phys. Rev. A **49**, 3 (1994)

[74] R. A. Horn, C. R. Johnson, *Matrix Analysis* (Cambridge University Press, 1985)

[75] V. V. Dodonov, J. Opt. B: Quantum Semiclass. Opt. **4**, S98 (2002)

[76] J. Williamson, Am. J. Math. **58**, 141 (1936); V. I. Arnold, *Mathematical Methods of Classical Mechanics* (Springer-Verlag, New York, 1978), Appendix 6.

[77] L. D. Landau, E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Pergamon Press, 1991)

[78] L. Heaney, J. Anders, Phys. Rev. A **80**, 032104 (2009)

[79] L. Heaney, Theory of Quantum Computation, Communication, and Cryptography Lecture Notes in Computer ScienceVolume **6519**, 2011, pp 175-186

[80] L. Heaney, J. Anders, Phys. Rev. Lett. **103**, 200502 (2009)

[81] L. Heaney, J. Anders, V. Vedral, arXiv:quant-ph/0607069 (2007)

[82] R. Simon, Phys. Rev. Lett. **84**, 2726 (2000)

[83] Lu-Ming Duan *et. al.*, Phys. Rev. Lett. **84**, 2722 (2000)

[84] E. Shchukin, W. Vogel, Phys. Rev. Lett. **95**, 230502 (2005)

[85] C. N. Gagatsos, A. I. Karanikas, G. I. Kordas, arXiv:quant-ph/1207.0303v2 (2012)

[86] C. Simon, Phys. Rev. A **66**, 052323 (2002)

[87] J. Goold, *et. al.* Phys. Rev. A **80**, 022338 (2009)

[88] D. Kaszlikowski *et. al.* arXiv:quant-ph/0601089v3 (2006)

[89] L. Heaney, arXiv:quant-ph/0711.0942v1 (2007)

[90] B. Reznik, Foundations of Physics **33**, 1 (2003)

[91] D. Kaszlikowski, V. Vedral, arXiv:quant-ph/0606238v1 (2006)

[92] A. Retzker *et. al.*, Phys. Rev. Lett. **94**, 050504 (2005)

[93] G. De Chiara *et. al.*, New J. Phys. **8** 95 (2006)

[94] L. Heaney *et. al.*, Phys. Rev. A **76**, 053605 (2007)

[95] G. Vidal, R. F. Werner, Phys. Rev. A **65**, 032314 (2002)

[96] S. Hill and W. K. Wootters, Phys. Rev. Lett. **78**, 26 (1997)

[97] W. K. Wootters, Phys. Rev. Lett. **80**, 10 (1998)

[98] R. M. Ziff *et. al.*, Phys. Rep. **32**, 169 (1977)

[99] H. D. Politzer, Phys. Rev. A **54**, 5048 (1996)

[100] S. Giorgini *et. al.*, Phys. Rev. Lett. **80**, 5040 (1998)

[101] F. London, Phys. Rev. **54**, 947 (1938)

[102] L. Pitaevskii, S. Stringari, *Bose-Einstein Condensation* (Oxford Science Publications, 2003)

[103] A. J. Leggett, *Quantum Liquids: Bose condensation and Cooper pairing in condensed-matter systems* (Oxford University Press, 2006)

[104] A. Recati *et. al.*, Phys. Rev. Lett. **94**, 040404 (2005)

[105] R. B. Diener *et. al.*, Phys. Rev. Lett. **89**, 070401 (2002)

[106] N. Schlosser *et. al.*, Nature (London) **411**, 1024 (2001)

[107] R. Dumke *et. al.*, Phys. Rev. Lett. **89**, 097903 (2002)

[108] I. H. Deutsch, P. S. Jessen, Phys. Rev. A **57**, 3 (1998)

[109] C. Chin *et. al.*, Rev. Mod. Phys. **82**, 1225b•“1286 (2010)