COMPLEMENTARITY OF QUANTUM CORRELATIONS

RAVISHANKAR RAMANATHAN
(B.Eng. (Hons), NTU)
(M.Sc., NUS)

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Declaration

I hereby declare that this thesis is my original work and it has been written by me in its entirety. I have duly acknowledged all the sources of information which have been used in the thesis.

This thesis has not been submitted for any degree in any university previously.

R.Ravishankar

Ravishankar Ramanathan
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Contents

Summary

Quantum theory differs from the classical theories of Nature in several respects. The more salient of these, such as the presence of entangled quantum states, the violation of Bell inequalities that implies a lack of the local realistic paradigm in Nature, the closely related contextuality of measurement results, the fundamental indistinguishability of quantum particles, and the impossibility of perfect cloning of quantum states have given rise to the burgeoning field of quantum information and computation, where these features are put to good use in performing information processing tasks unachievable in the classical context.

In this thesis, we study the correlations in quantum states that lead to these remarkable properties and examine them in turn, with a focus on one particular aspect of the correlations, namely their complementarity or monogamous nature. The monogamy of quantum correlations, which qualitatively implies that strong correlations between two quantum systems lead to their weak correlations with other systems, has a number of consequences. We begin with a study of the optimal cloning problem in quantum theory, a problem with ramifications as far as quantum cryptography, and derive its solution in the scenario of obtaining a given number of copies of an unknown quantum state. As a by-product, we obtain a monogamy relation for entanglement, the basic resource in quantum information. A method is then introduced for the derivation of monogamy relations for Bell inequality violations in the ubiquitous scenario of qubit Bell inequalities involving two measurement settings per party. A significant consequence of the Bell monogamy relations is then demonstrated, namely the emergence of a local realistic description for the correlations in everyday macroscopic systems.

A closely related concept to local realism is contextuality, a phenomenon which precludes the assignment of outcomes to measurements before they are performed. We analytically demonstrate the minimal number of measurements required to reveal the contextuality of the simplest such system, the qutrit, and derive contextual inequalities analogous to Bell inequalities based on the information-theoretic concept of entropy. Monogamy relations are derived for contextuality based on the principle of no-disturbance, a generalization of the principle of no-signaling to single systems. Macroscopic systems are shown to admit non-contextual description for the feasible measurements that can be performed on them, a result that coupled with the local realistic description of the correlations in these systems, suggests the possibility of their classical description. Finally, we turn to the study of indistinguishable composite particles in Nature, and investigate the role of entanglement and its monogamy in the display of fermionic and bosonic behavior by such particles, utilizing the tools of quantum information to tackle this old and important question. An understanding of these principal features of quantum theory is, we believe, important in the march towards its utilization in computation and information processing.

List of Figures

Publications

This thesis is based on the following publications:

1. **Optimal Cloning and Singlet Monogamy:**
   Alastair Kay, Dagomir Kaszlikowski and Ravishankar Ramanathan,
   Physical Review Letters, **103** 050501, arXiv/quant-ph: 0901.3626 (2009).

2. **Correlation complementarity yields Bell monogamy relations:**
   Pawel Kurzynski, Tomasz Paterek, Ravishankar Ramanathan, Wieslaw Laskowski and Dagomir Kaszlikowski,
   Physical Review Letters **106** 180402, arXiv/quant-ph: 1010.2012 (2011).

3. **Local Realism of Macroscopic Correlations:**
   Ravishankar Ramanathan, Tomasz Paterek, Alastair Kay, Pawel Kurzynski and Dagomir Kaszlikowski,
   Physical Review Letters **107** 060405, arXiv/quant-ph: 1010.2016 (2011).

4. **Entropic test of quantum contextuality:**
   Pawel Kurzynski, Ravishankar Ramanathan and Dagomir Kaszlikowski,
   Physical Review Letters **109** 020404, arXiv/quant-ph: 1201.2865 (2012).

5. **Generalized monogamy of contextual inequalities from the no-disturbance principle:**
   Ravishankar Ramanathan, Akihito Soeda, Pawel Kurzynski, Dagomir Kaszlikowski,
   Physical Review Letters **109** 050404 , arXiv/quant-ph: 1201.5836 (2012).

6. **Experimental undecidability of macroscopic quantumness:**
   Pawel Kurzynski, Akihito Soeda, Ravishankar Ramanathan, Andrzej Grudka, Jayne Thompson and Dagomir Kaszlikowski, arXiv/quant-ph: 1111.2696 (2011).

7. **Criteria for two distinguishable fermions to form a boson:**
   Ravishankar Ramanathan, Pawel Kurzynski, Tan Kok Chuan, Marcelo F. Santos and Dagomir Kaszlikowski,
   Physical Review A (Brief Reports) **84** 034304, arXiv/quant-ph: 1103.1206 (2011).

8. **Particle addition and subtraction as a test of bosonic quality:**
   Pawel Kurzynski, Ravishankar Ramanathan, Akihito Soeda, Tan Kok Chuan and Dagomir Kaszlikowski,
   New Journal of Physics **14** 093047 (2012), arXiv/quant-ph: 1108.2998 (2011).

9. **Optimal Asymmetric Quantum Cloning:**
   Alastair Kay, Ravishankar Ramanathan and Dagomir Kaszlikowski,
   arXiv/quant-ph: 1208.5574 (2012).

Chapter 1

Introduction

Quantum Theory is the most accurate description of Nature we know today. Originally devised to explain certain classically perplexing phenomena such as blackbody radiation and the stability of electron orbitals in atoms, it has since been unequivocally successful in describing the behavior of subatomic particles, the formation of atoms and molecules in chemistry, the interaction of light and matter, and many such intriguing aspects of Nature. A number of modern technological inventions such as the laser, the diode and the transistor, the electron microscope etc. have also been built using its principles. Yet, it is an acknowledged fact that the worldview imposed by the theory is truly bizarre. Quantum theory incorporates a number of strange features such as entanglement, contextuality, indistinguishable particles and violates certain common sense principles such as local realism. This thesis is primarily concerned with these features of quantum mechanics that distinguish it from all classical theories. At the same time, we shall be concerned with the practical applications of these aspects of quantum mechanics in information theoretic scenarios.

The most radical departure of quantum mechanics from classical physics is the lack of the so-called “local realism” in the theory. This puzzling feature of quantum mechanics was first brought to light in a classic paper by Einstein, Podolsky and Rosen (EPR) [1] in 1935. This extremely well-cited paper may, with good justification, be argued to be the founding paper of the field of quantum information (the sister field of quantum computation could be said to have begun more recently with the ideas of Feynman in [2]). Quantum mechanics is well-known to be a probabilistic theory, providing answers to questions such as the position of an electron or its spin only in terms of probabilities. This non-deterministic character of the theory is further exacerbated by the fact that it does not incorporate the intuitive feature of “realism”.

Realism is the idea that objects have definite states with predetermined outcomes for all their measurable properties such as position, momentum, spin etc. In contrast, the outcomes of quantum mechanical measurements are brought about at the instant of measurement. Moreover, the knowledge of one property such as the spin of a particle in a particular direction renders the outcomes of complementary properties such as spins in other directions completely random. Thinking about the consequences of this fact lead Einstein to ask deep questions such as “Do you really think the Moon is not there when nobody looks?” (in conversation with Abraham Pais [3]). This lack of realism is a fundamental departure from classical theories such as Newtonian mechanics and Electromagnetism, where the measurements play a more passive role and the objects have well-defined properties (such as charge, mass, position, momentum) irrespective of whether those properties are measured. A further departure from classical physics concerns the apparent non-local character of the theory.

Locality (a notion inspired by Einstein’s Theory of Relativity) states that an action such as measurement of a particle’s position or momentum or other degrees of freedom, performed at a particular location should not influence the outcomes when particles in spatially distant locations are measured. By means of a characteristic thought experiment and clear reasoning, EPR argued that either quantum mechanics is an incomplete theory in so far as it fails to account for the simultaneous existence of certain elements of reality such as the spin of a particle in multiple directions, or that it violated the principle of a finite propagation speed for physical effects (a view completely untenable in light of the success of the Theory of Relativity). While EPR did not refute the accuracy of quantum mechanics and its success as a physical theory of Nature, they suggested that it ought to be completed by a more refined physical theory which incorporated certain “hidden variables”. These would then allow for the simultaneous existence of elements of reality forbidden in quantum theory.

Discussions such as the above were relegated to the status of a philosophical debate by many researchers interested in calculating the intriguing experimental implications of the theory, until the question whether Nature is local realistic in the EPR sense was precisely made experimentally testable in 1964 by John Bell [4]. Bell formulated an algebraic inequality using the probabilities of measurement outcomes and the correlations between outcomes in spatially separated locations. This inequality would have to be satisfied in any physical theory incorporating local realism. On the contrary, there exist certain “entangled states” in quantum theory for which the correlations of measurement results would violate the inequality. Bell’s theorem which is arguably one of the most profound theorems in science rendered it a question for experiment to decide if Nature obeyed the constraints of local realism or not.

All the experiments performed so far are in favor of quantum mechanics showing that a local realistic description of microscopic systems is untenable. Although none of the experiments so far have fulfilled all the requisite conditions for the exclusion of local realistic theories (a huge effort is on to conduct the definitive experiment that would close all the possible loopholes), most researchers are convinced that the violation of Bell inequalities seen in the laboratory indicate the correctness and completeness of quantum mechanics in the EPR sense. In fact, this question has several important practical implications, as it is now known that the violation of Bell inequalities guarantee a quantum advantage for information theoretic protocols such as quantum cryptography [5], randomness amplification [6], and in the non-triviality of communication complexity [7].

One of the results set forth in this thesis is that while entangled states of microscopic systems can violate Bell inequalities, the macroscopic world we experience *can* be described in terms of local realism. We shall see that the crucial aspect of the argument is that the feasible measurements on macroscopic systems (of the order of an Avogadro number of particles) are limited, and one cannot address every microscopic constituent of these systems. This is well known as one of the central features in the statistical mechanical description of these systems [8]. The limited class of measurements performable on a macroscopic system coupled with an intriguing property of Bell inequalities called the monogamy of their violation leads to the local hidden variable description of these systems.

Developments in Bell inequalities go hand-in-hand with the theory of entanglement that has become an important subfield of quantum information with a lot of well-established results (although open questions remain in the regime of multiple particle entanglement). While entangled states are necessary for the violation of Bell inequalities, entanglement is also useful as a fundamental resource in several quantum information protocols such as quantum teleportation, dense coding of information, etc. For pure entangled states of two or more composite systems, the state of the global system is completely known while the properties of the individual systems remain indeterminate, a truly quantum feature with no classical parallel.

The notion of local realism that applies to composite systems can also be generalized to the domain of single systems by the idea of "contextuality". Non-Contextuality is the common sense hypothesis that the outcomes of measurements of physical quantities are independent of the measurement arrangement devised to find them. The first rigorous result in this field was the Kochen-Specker theorem [9] which can be understood as a complement to Bell's theorem. This theorem excludes the possibility of non-contextual hidden variable theories representing quantum systems whose dimension is greater than two. In other words it excludes the notion that quantum mechanical observables are elements of physical reality whose values are present before the measurement in such a manner that the knowledge of one influences the outcomes of others. The fact that quantum mechanics is a contextual theory has been exploited in some cryptographic scenarios [10] and efforts are underway to find the minimal set of measurements that show contextuality for given system dimensions. In this thesis, we derive contextual inequalities analogous to Bell inequalities using the information-theoretic notion of entropy. We also find the intriguing feature of complementarity or monogamy in contextuality; when a particular set of measurements reveals contextuality a complementary set of measurements is forced to become non-contextual even though these complementary measurements can themselves reveal contextuality when the first set of measurements is non-contextual. Moreover, we also investigate the possibility of macroscopic contextuality, the question whether macroscopically feasible measurements can exhibit contextuality.

Another cornerstone of the theory of quantum information concerns the replication of the information stored in quantum systems. While classical bits may be arbitrarily copied, the No-Cloning Theorem in quantum mechanics [11] states that the state of a quantum system cannot be duplicated perfectly. This fundamental theorem lies at the heart of some quantum communication protocols, in particular quantum cryptography. It also gives rise to the optimal cloning problem, which is the question of how well a given arbitrary quantum state can be copied. This well-studied question with wide implications for the transfer of quantum information, is one of the topics we study in this thesis. As we shall show, the case of replicating one copy of an arbitrary quantum state into N copies can be solved exactly. Several other cases such as the copying from M to N, the copying of a restricted set of states etc. remain in need of exact solutions. Intriguingly, we shall also see that the cloning problem is related to the phenomenon of monogamy of entanglement. This latter property that states that the more entangled a spin is with another, the less entangled it can be with other spins, has found applications in even condensed matter scenarios in bounding the properties of certain Hamiltonians.

An aspect of quantum mechanics that has gained attention in quantum information theory with the experimental realization of the Bose-Einstein condensate is the possibility of truly indistinguishable particles, a feature which has no classical analog. Protocols for estimation of quantum states have been built using indistinguishability [12], and there is hope that more protocols will exploit this truly quantum feature to gain advantage over classical algorithms. Indistinguishable particles are classified broadly into the two categories of Fermions and Bosons which obey the Fermi-Dirac and Bose-Einstein statistics respectively. Identical fermions are forbidden from occupying the same quantum state by the Pauli exclusion principle, while for bosons, the occupation of the same state is encouraged by a bosonic enhancement factor over classical distinguishable particles. Many of the particles in Nature are composite, being composed of elementary fermions or bosons. The dependence of the bosonic and fermionic behavior of these composite particles on the quantum states of their elementary constituents, in particular on the necessity of entanglement in these states, has recently received attention. In a chapter on indistinguishable composite particles, we shall investigate this question thoroughly from a mathematical as well a physical perspective.

This thesis thus flows as an investigation of several truly quantum features that make the theory appealing from both a fundamental and an application oriented viewpoint. In particular, we discuss in turn, (i) solutions for the optimal cloning problem and entanglement monogamy, (ii) the monogamy of Bell inequality violations, (iii) the appearance of a local realistic description for macroscopic systems as a consequence of these, (iv) inequalities to test contextuality and monogamy relations for contextual inequalities, (v) the possibility of macroscopic contextuality, and finally (vi) the role of entanglement in indistinguishable composite particle behavior. A common thread runs through all these topics, namely the study of quantum correlations focusing in particular on the aspect of complementarity or monogamy of the correlations. All concepts necessary for the understanding of the chapters are explained in the introduction to the chapters and only basic knowledge of quantum theory is assumed. It is hoped that the results presented here and in particular the open questions listed at the end of each topic, shall spur much fruitful research into these intriguing aspects of Nature.

Chapter 2

Optimal Cloning and Entanglement Monogamy

One of the most striking aspects of the quantum encoding of information regards the possibility of copying such information. When information is encoded in the state ψ of a quantum system, the process of replicating the state $\psi \to \psi \otimes \psi$ is called "cloning". The well-known $no - cloning$ theorem [11] forbids the cloning of an arbitrary quantum state, in particular no quantum operation exists that can clone arbitrary non-orthogonal states. The no-cloning theorem is one of the cornerstones of quantum theory, and has been related to other fundamental ideas such as the principle of no-signaling [13] and the uncertainty relations. The quantitative link to the question of estimating the state of a quantum system has been established [14]. Apart from the intrinsic theoretical interest, the no-cloning theorem has also found application in quantum cryptography [15] where it enables detection of attempts by an adversary to copy the information on a communication channel. While the no-cloning theorem is now well established, the question of the extent to which an unknown quantum state can be copied has been the subject of intensive research, excellent reviews of which can be found in [16, 17].

The optimal cloning of discrete quantum states began with the idea of the Buzek-Hillery quantum cloning machine which obtains two identical copies of a given unknown spin-1/2 particle's (qubit) state [18]. This has been extended to $M \to N$ cloning [19] where starting from M copies of the same unknown quantum state, the task is to produce N output copies of as high a quality as possible. While the original cloning machines were symmetric, in the sense that all output copies had the same fidelity, this has also been extended to asymmetric cloning [20]. In this latter task, not all copies need to have the same quality, some output clones can be designed to have higher fidelities at the expense of others. The original cloning machines were also designed to clone all input pure states of a given dimension, this is termed "universal cloning": for any Hilbert space dimension, the unknown input state is equally likely to be any possible pure single qudit state, i.e.

drawn randomly from the uniform Haar distribution. On the other hand, when there is some prior knowledge of the distribution of the states to be cloned, better strategies can be devised, this task is known as state-dependent cloning. In this regard, there are several well-known instances. The first of these is called "equatorial cloning": for $d = 2$, the state of the qubit is known to be drawn from the set of states in the equator of the Bloch sphere, $(|0\rangle + e^{i\phi}|1\rangle)/\sqrt{2}$ and any angle ϕ in the range 0 to 2π is equally likely. Another well-studied instance is known as "phase-covariant" cloning: for $d = 2$, the state of the qubit is known to be drawn from the set $\cos\theta|0\rangle + \sin\theta e^{i\phi}|1\rangle$ with a probability distribution that is independent of the parameter ϕ. In addition to the studies on state-dependent cloning, the issue of "economic" cloning has also been addressed. If the optimal cloning machine can be implemented by an unitary operation without any ancillary systems, the cloner is said to be economical, otherwise it is not [21, 22]. The presence or absence of the ancilla significantly alters the implementation of the cloner experimentally, the economic cloner being simpler to control and less sensitive to decoherence effects.

In this chapter, we concentrate on cloning as being an intriguing aspect of quantum information. We begin with the no-cloning theorem, and explain its relation to the principle of no-signaling, monogamy of entanglement and the state estimation problem. We then study the universal quantum cloning of qudits from 1 copy to an arbitrary number (N) of copies for general asymmetries and present a general solution for the optimal cloning. In doing so, we derive a monogamy relation for the maximally entangled fraction (singlet fraction) of quantum states defined as the overlap of the given state with a maximally entangled state. We then show how this singlet monogamy relation may be applied in condensed matter scenarios, such as in deriving a bound to the ground state energy of some Hamiltonians. We end with a discussion on possible extensions of the proposed methods and open questions. The material on universal cloning is a detailed account of [23] while the results on state-dependent qubit cloning have been put forth in [24], both joint works of the author and collaborators.

2.1 No-Cloning Theorem

Formally, the no-cloning theorem [11] states that no quantum operation can perfectly duplicate an arbitrary quantum state. The proof of this statement follows from the linearity and unitarity of quantum theory and can be seen as follows (proofs of the theorem can be found for e.g. in [16]).

The most general quantum evolution is by a Completely Positive Trace Preserving (CPTP) map. Any such map can be implemented by adding an auxiliary system known as the ancilla to the system under study, and then letting the whole system plus ancilla state undergo unitary evolution, finally tracing out the ancilla. Letting $|\psi\rangle$ denote the state of the system that one would like to clone, and $|A\rangle$ denote the ancilla, the cloning process is represented as

$$|\psi\rangle \otimes |B\rangle \otimes |A\rangle \rightarrow |\psi\rangle \otimes |\psi\rangle \otimes |A'\rangle$$

Here $|B\rangle$ denotes the blank state on which the cloned copy appears and $|A'\rangle$ denotes the state of the ancilla after the unitary evolution. For two orthogonal states $|\psi\rangle$ and $|\psi^{\perp}\rangle$ the above process works as

$$\begin{aligned} |\psi\rangle \otimes |B\rangle \otimes |A\rangle &\rightarrow |\psi\rangle \otimes |\psi\rangle \otimes |A'\rangle \\ |\psi^{\perp}\rangle \otimes |B\rangle \otimes |A\rangle &\rightarrow |\psi^{\perp}\rangle \otimes |\psi^{\perp}\rangle \otimes |A''\rangle. \end{aligned}$$

Now while the linearity of quantum theory requires that

$$(|\psi\rangle + |\psi^{\perp}\rangle) \otimes |B\rangle \otimes |A\rangle \rightarrow |\psi\rangle \otimes |\psi\rangle \otimes |A'\rangle + |\psi^{\perp}\rangle \otimes |\psi^{\perp}\rangle \otimes |A''\rangle \tag{2.1}$$

we would like the actual output of the cloning process for the (unnormalized) state $(|\psi\rangle + |\psi^{\perp}\rangle)$ to be

$$(|\psi\rangle + |\psi^{\perp}\rangle) \otimes |B\rangle \otimes |A\rangle \rightarrow (|\psi\rangle + |\psi^{\perp}\rangle) \otimes (|\psi\rangle + |\psi^{\perp}\rangle) \otimes |A'''\rangle$$

which is clearly not the same as the state generated in Eqn. (2.1) as can be seen by simple expansion. The above argument based on the linearity of quantum theory shows that while cloning works for states of an orthonormal basis, one cannot clone an arbitrary quantum state in general. Alternative proofs based on the unitarity of state evolution in quantum theory can also be found [16].

The no-cloning theorem is at the heart of quantum cryptographic schemes where an eavesdropper cannot obtain a copy of any shared data without disturbing it in a detectable manner, and this is guaranteed by the laws of physics rather than assumptions on the difficulty of computation as in the classical case. There are also many fundamental concepts in quantum information theory that are related to no-cloning such as quantum state estimation, state discrimination, the no-broadcasting theorem (a generalization of no-cloning to mixed quantum states), quantum disentanglement etc. As regards state estimation, we can understand that if a quantum cloner existed, we could prepare many copies of an unknown quantum state $|\psi\rangle$ and measure the average values of several observables on the copies, thereby determining the state accurately. Moreover, this procedure would also allow unambiguous discrimination of non-orthogonal quantum states.

More interestingly (what was one of the original motivations behind the theorem), one could also use a quantum cloner to transmit information faster than light leading to a violation of the no-signaling principle (a consequence of the theory of relativity). For instance, we can imagine a protocol in which a source produces two qubits in the singlet state $|\psi_-\rangle = \frac{1}{\sqrt{2}}(|0_z 1_z\rangle - |1_z 0_z\rangle) = \frac{1}{\sqrt{2}}(|0_x 1_x\rangle - |1_x 0_x\rangle)$ and sends one particle each to two spatially separated parties, Alice and Bob. If Alice had a quantum cloner, Bob could use it to transmit a message to Alice superluminally as follows [16]. First, he encodes his message in a binary string. He then chooses to measure his qubit in the x or z direction, depending on whether he is transmitting bit 0 or bit 1. In either case, quantum theory tells us that Alice's qubit will collapse to the completely mixed state $\rho_A = \frac{1}{2}(|0_z\rangle\langle 0_z| + |1_z\rangle\langle 1_z|) = \frac{1}{2}(|0_x\rangle\langle 0_x| + |1_x\rangle\langle 1_x|)$ and so normally Alice does not know the bit that Bob is trying to send to her. If however, Alice had a quantum cloner, she can use it to clone her qubit to the state $\rho'_A = \frac{1}{2}(|0_z^{\otimes N}\rangle\langle 0_z^{\otimes N}| + |1_z^{\otimes N}\rangle\langle 1_z^{\otimes N}|) \neq \frac{1}{2}(|0_x^{\otimes N}\rangle\langle 0_x^{\otimes N}| + |1_x^{\otimes N}\rangle\langle 1_x^{\otimes N}|)$. In this situation, as N gets larger, the two states get more orthogonal and distinguishable, and Alice can determine the bit that Bob is transmitting with arbitrary precision. By forbidding such protocols, the no-cloning theorem prevents a contradiction between quantum theory and the theory of relativity.

Another fundamental concept of quantum mechanics, entanglement, is also linked to the no-cloning theorem. In particular, it is known that it is impossible for a single spin to be maximally entangled with two other spins simultaneously. This concept of monogamy of entanglement which has an impact on fields as diverse as superconductivity [25], has been difficult to quantify so far. A strict inequality relation has only been proven for the tangle [26, 27] (the precise definition of the tangle is provided in Section (2.4)), and this particular measure is not a naturally applicable quantity in other branches of physics. Nevertheless, this inequality has proven to be useful for bounding ground state energies of some condensed matter systems. Heuristically, the link between cloning and monogamy can be seen by considering a process involving three entangled spins. One follows a teleportation protocol [29] with an unknown state, targeting spin 0. Copies of the unknown state appear on the other two spins, and the quality of the copies depends on how much entanglement was in the original state, the more entanglement between say spins 0 and 1, the better the quality of the copy of the unknown state at spin 1. This leads to the conclusion that if a particular quality of cloning is impossible (in particular if the unknown state cannot appear perfectly at both spins 1 and 2), a certain degree of entanglement must be impossible (no state can have maximal entanglement between spins 0 and 1 as well as between spins 0 and 2). The no-cloning theorem is thus intrinsically related to the phenomenon of monogamy of entanglement, see Fig. (2.1). In the figure, the cloning of an unknown input state $|\psi_{in}\rangle$ into two copies following the teleportation procedure is shown. The quality of the two outputs denoted by F_1 and F_2 depend on the entanglement shared by the input port 0 with each of the two output ports 1 and 2, denoted by $p_{0,1}$ and $p_{0.2}$, respectively.

As seen before, the no-cloning theorem leads naturally to the question that if perfect cloning of an unknown quantum state is not possible, what are the optimal imperfect copies that one can produce? The Buzek-Hillery $1 \rightarrow 2$ universal qubit cloning machine is

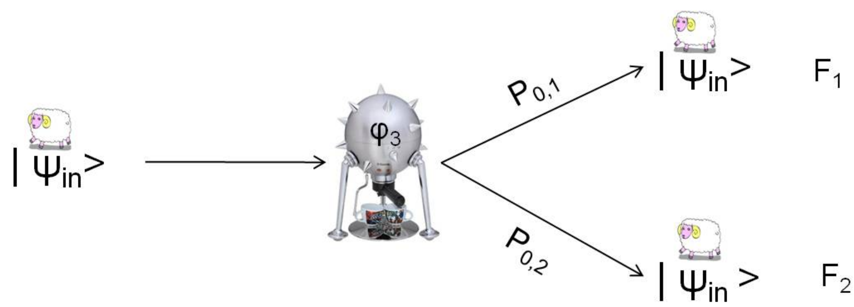

Figure 2.1: The relation between the no-cloning theorem and the monogamy of entanglement is illustrated via a telecloning process. The cloning of an unknown input state $|\psi_{in}\rangle$ into two copies following the teleportation procedure shows that the quality of the copies at the two outputs denoted by F_1 and F_2 depend on the entanglement shared by the input port 0 with each of the two output ports 1 and 2, denoted by $p_{0,1}$ and $p_{0,2}$.

known to be optimal [14], in the sense that it maximizes the average fidelity between the input and output states. The fidelity is a measure of the quality of the copy and is given by $F = \langle\psi|\rho|\psi\rangle$ with $|\psi\rangle$ the state to be copied and ρ describing the density matrix of the approximate copy. The general $1 \to N$ universal qudit cloning problem will be the main focus of this chapter.

2.2 The Choi-Jamiołkowski isomorphism

We begin with an explanation of the main tool used in the solution of optimal cloning tasks, the well-known Choi-Jamiołkowski isomorphism. This formalism is used in general to find how well a particular state transformation task can be achieved by a quantum process, i.e., a completely positive map [30].

The scenario is as follows. We are given one of a set of N states $|\psi_i\rangle$ $(i = 1, \ldots, N)$, and we are required to perform a particular transformation of the state, without knowing exactly which of the N states we have been given. The required transformation may not be achievable exactly within the quantum formalism (such as is the case for a perfect cloning task), but is best approximated within the theory by a completely positive, trace preserving map $\mathcal{E}$ that transforms input state $|\psi_i\rangle$ into $\mathcal{E}(|\psi_i\rangle)$. The success of the state transformation task is then measured by a fidelity given by

$$F = \frac{1}{N} \sum_i tr \left(\mathcal{M}_i \mathcal{E}(|\psi_i\rangle \langle\psi_i|) \right).$$

Here $\mathcal{M}_i$ are positive operators ($\mathcal{M}_i \geq 0$) satisfying $\|\mathcal{M}_i\| \leq 1$ so that F is indeed a fidelity taking values between 0 and 1. If the fidelity takes value 1, we infer that the map $\mathcal{E}$ has perfectly implemented the required state transformation for all the specified input states. As a simple example, consider the case when we are required to transform the states $|\psi_i\rangle$ into states $|\phi_i\rangle$, in which case we simply define $\mathcal{M}_i = |\phi_i\rangle\langle\phi_i|$. In the problem of the $1 \to N$ cloning transformation where the quality of cloning is measured by local single copy fidelities, we take $\mathcal{M}_i = \sum_{n=1}^{N} \alpha_n |\psi_i\rangle\langle\psi_i|_n$ and if the quality is measured by a global fidelity we take $\mathcal{M}_i = |\psi_i\rangle\langle\psi_i|^{\otimes N}$.

The fidelity can now be rewritten in a manner that yields definite upper bounds. This is accomplished by the isomorphism as follows. Since $\mathcal{E}$ is a completely positive map, its operation on a subsystem O of a bipartite entangled state (entangled between input system I and output O) is well defined. Let us denote the maximally entangled state of interest as

$$|B\rangle = \frac{1}{\sqrt{d}} \sum_{n=0}^{d-1} |\phi_n\rangle_I |\phi_n\rangle_O ,$$

where the basis states $|\phi_n\rangle$ $(n = 0, \ldots, d-1)$ span the subspace occupied by the set of input states $|\psi_i\rangle$ (which have dimension d). The action of the composite map, composed of the identity on the input space and the desired map $\mathcal{E}$ on the output space of the maximally entangled state gives us the output χ_{IO},

$$\mathbb{1}_I \otimes \mathcal{E}(|B\rangle\langle B|)_O = \chi_{IO}.$$

The condition that $\mathcal{E}$ be trace preserving then implies that $tr(\chi_{IO}) = \langle B|B\rangle = 1$. In fact, as long as the map is not trace increasing so that $tr(\chi_{IO}) \leq 1$, our conclusions will be valid since we are interested in finding an upper bound to the fidelity of state transformation. This fidelity can now be evaluated as

$$F = \frac{d}{N} \sum_i tr\left(\chi_{IO}(|\psi_i\rangle\langle\psi_i|_I^T \otimes \mathcal{M}_i)\right),$$

where the superscript T denotes transposition. If we define a matrix R as

$$R = \frac{d}{N} \sum_i |\psi_i\rangle\langle\psi_i|_I^T \otimes \mathcal{M}_i,$$

then we obtain

$$F = tr(R\chi_{IO}) \leq tr(\chi_{IO}) r_{\max} \leq r_{\max} \tag{2.2}$$

where $r_{\max}$ is the maximum eigenvalue of matrix R. We thus arrive at the important conclusion that the maximum fidelity achievable within the quantum theory of a given state transformation task is bounded by the maximum eigenvalue of a suitably formulated matrix R. The fact that the state transformation problem has been transformed into the problem of finding the maximum eigenvalue of a matrix is interesting and highly useful. Even if the matrix R proves to be difficult to diagonalize exactly, one can use many techniques (borrowed for instance from condensed matter physics) to bound the achievable fidelities. One example of such a technique that has been used in finding bounds on ground state energies of condensed matter systems is to upper bound the norm of the matrix by the sum of the norms of the constituent terms [31].

2.2.1 Condition for achieving the maximum fidelity by a CP map

From the considerations above, we see that the maximum eigenvector, $|\Psi\rangle$, of the matrix R defines the optimal strategy if it can be realized. If this state is unique, consider it as a pure bipartite state between the subsystems I and O. This state can be written in the Schmidt basis [32] as

$$|\Psi\rangle = \sum_{n=0}^{d-1} \beta_n |\phi_n\rangle_I |\lambda_n\rangle_O .$$

We will have occassion to study the Schmidt basis when we study entanglement in detail in a later chapter on composite particles. For the moment, we will simply use the fact that when the Schmidt coefficients are given by $\beta_n^2 = \frac{1}{d}$, the state is maximally entangled across the partition between input and output and can be implemented by a unitary U, defined as

$$U |\phi_n\rangle = |\lambda_n\rangle .$$

Here the relevant Hilbert spaces are extended as necessary so that they have the same size. In this instance, the optimal strategy is called economical, meaning that one does not require an ancilla for the operation to be implemented. In fact, even if the maximum eigenvector is not unique, as long as there exists a superposition of the maximum eigenvectors that is maximally entangled, the optimal map can be implemented as a unitary and is therefore economical.

More generally, if there exists a mixture of the maximum eigenvectors of R, ρ_R, such that $tr_O\rho_R$ is maximally mixed (given by $\frac{1}{d}\mathbb{1}_I$), then this can be implemented as a CP map or, equivalently, a unitary operator over a larger Hilbert space, in which case the operation is no longer economical. The condition for implementation of the state transformation task optimally by a CP map is therefore

$$tr_O\rho_R = \tfrac{1}{d}\mathbb{1}_I.$$

That this condition is sufficient is seen by recognizing that one can add an auxiliary Hilbert space to purify ρ_R. The overall pure state then defines a unitary as in the previous case although this operation is not economical. That this condition is also necessary is seen by writing the optimal CP map using the Kraus decomposition [32] as

$$\mathcal{E}(\rho) = \sum_i A_i \rho A_i^\dagger$$

where $\sum_i A_i^\dagger A_i = \mathbb{1}$. We then find that

$$\rho_R = \mathbb{1}_I \otimes \mathcal{E}_O(|B\rangle\langle B|) = \sum_i A_i^O |B\rangle\langle B|_{IO} A_i^{O\dagger}.$$

And upon performing the partial trace over O, we obtain

$$tr_O\rho_R = tr_O\left(\sum_i A_i^\dagger A_i |B\rangle\langle B|_{IO}\right),$$

which can be reduced using the completeness relation for the Kraus operators $\sum_i A_i^\dagger A_i = \mathbb{1}$ to $tr_O\rho_R = \frac{1}{d}\mathbb{1}$.

As a final remark we mention that the optimal strategy can also be implemented by teleporting the input state onto spin I of a resource state which could be either $|\Psi\rangle$ or the purification of ρ_R. The different measurement results of teleportation can be corrected for by action on the output space (and its extension if required). This gives rise in the case of the cloning task to the well-known telecloning protocols [33].

2.2.2 Application to cloning quantum states

The potentially powerful formalism described above is now used in the problem of the optimal cloning of quantum mechanical states. In the quantum cloning process, we start with an unknown quantum state $|\psi\rangle$ of Hilbert space dimension d, and aim at producing N copies of the state. It is known that this state is drawn from a set of possible states Σ with distribution $f(\psi)$ that is normalized as

$$\int_\Sigma f(\psi)d\psi = 1.$$

Dividing the output space O into N qudits labeled 1 to N, our aim is to optimize the quality of the N different copies to be produced. There are different figures of merit that can be applied to cloning (i.e. different definitions of the $\mathcal{M}_i$ defined in the previous section). The simplest figure of merit is the *global fidelity*, for which $\mathcal{M}_i = |\psi_i\rangle\langle\psi_i|^{\otimes N}$. The solution to the cloning problem in terms of the global fidelity is known [34] and will not concern us in the rest of the chapter. Instead, we consider the *single copy fidelity*, in which we take the global output state $\rho_{1\ldots N}$, and assess the fidelity of a single copy on a given site n, $F_n = tr(|\psi_i\rangle\langle\psi_i|_n \rho_{1\ldots N})$. To this end, we define

$$\mathcal{M}_i = \sum_{n=1}^N \alpha_n \mathbb{1}_1 \otimes \ldots \mathbb{1}_{n-1} \otimes |\psi_i\rangle\langle\psi_i|_n \otimes \mathbb{1}_{n+1} \otimes \cdots \otimes \mathbb{1}_N$$

where imposing $\sum_{n=1}^N \alpha_n = 1$ ensures that the $\mathcal{M}_i$ satisfy the required property $\|\mathcal{M}_i\| \leq 1$ in addition to $\mathcal{M}_i \geq 0$. In particular, $F = 1$ can still only be achieved if the output state is $|\psi_i\rangle^{\otimes N}$ for all inputs i. For generality, we assign different weights α_n to the different copies, emphasizing a possible desire for different qualities of output, although a common desire is equal qualities, $\alpha_n = 1/N$. The latter case is called optimal symmetric cloning while the general scenario is the optimal asymmetric cloning from 1 to N copies, the overall fidelity being given by the relation $\sum_n \alpha_n F_n = F$.

For the single copy fidelity, on which we henceforth concentrate exclusively, the matrix R is seen to be

$$R = \int_\Sigma f(\psi) d\psi \, |\psi\rangle \langle\psi|_I^T \otimes \sum_{n=1}^{N} \alpha_n \mathbb{1}_1 \otimes \ldots \mathbb{1}_{n-1} \otimes |\psi\rangle \langle\psi|_n \otimes \mathbb{1}_{n+1} \otimes \cdots \otimes \mathbb{1}_N \tag{2.3}$$

We are considering here cloning from a single copy of $|\psi\rangle$ so that the problem is $1 \to N$ cloning. This means that the dimension of the input Hilbert space I is exactly d, and the basis is simply $|i\rangle$ for $i = 0 \ldots d-1$.

2.3 Optimal $1 \to N$ Asymmetric Universal Qudit Cloning

When performing $1 \to N$ cloning, the aim is to transform a given input state $|\psi_{in}\rangle \langle\psi_{in}|$ into N copies $|\psi_{in}\rangle \langle\psi_{in}|^{\otimes N}$ with as high a fidelity as possible. For universal cloning, where no prior information about the input state is available, the distribution must be taken to be uniform, and $|\psi_{in}\rangle$ can be written as $U|0\rangle$, so that

$$R = \int dU \sum_{n=1}^{N} \alpha_n U^T \otimes U |00\rangle \langle 00|_{0,n} U^* \otimes U^\dagger.$$

Here the integration results in twirling [35] to give

$$R = \frac{1}{d(d+1)} \sum_{n=1}^{N} \alpha_n \left(\mathbb{1} + d |B_0\rangle \langle B_0|\right)_{0,n}. \tag{2.4}$$

Here, $|B_0\rangle = \sum_{i=0}^{d-1} |ii\rangle / \sqrt{d}$ denotes the maximally entangled state in d dimensions and tensoring with $\mathbb{1}$ on all other sites apart from n is implied in each term. For any given set of coefficients $\{\alpha_n\}$, this matrix can, in principle, be diagonalized and the solution to the universal cloning problem in terms of the optimal trade-offs between the different fidelities F_n can be found.

Using these, one can also derive a kind of entanglement monogamy relation as follows. One can define as an indicator of entanglement, the singlet fractions

$$p_{0,n} = \max_{U,V} \langle B_0| U \otimes V \rho_{0,n} U^\dagger \otimes V^\dagger |B_0\rangle$$

of the reduced states $\rho_{0,n}$ of a many-body state $|\Psi\rangle$, with U and V being arbitrary d-

dimensional unitary rotations (note that one may in fact use the symmetries of the maximally entangled state $|B_0\rangle$ to maximize over unitaries on one side only). The fact that the singlet fraction $p_{0,n}$ is intrinsically linked with the teleportation fidelity as $F_n = (p_{0,n}d+1)/(d+1)$ [36], implies that the trade-off relation for the fidelities elucidates the optimal trade-off between how much of a singlet a particular spin can share with all the others. In other words, one can recast the fidelity trade-off relation as a "singlet monogamy relation".

In this class of cloners, our method can be understood as wanting to maximize $F = \sum_n \alpha_n F_n = \sum_n \alpha_n (p_{0,n}d+1)/(d+1)$ under the constraint $\sum_n \alpha_n = 1$, which is equivalent to demanding the state $|\Psi\rangle$ which optimizes its overlap with $\sum_n \alpha_n (|B_0\rangle\langle B_0|_{0,n} d+1)/(d+1)$. That state must be the maximum eigenvector of R. To proceed with solving Eqn. (2.4), we propose an ansatz for the maximum eigenvector of R,

$$|\Psi\rangle = \sum_{n=1}^{N} \beta_n |B_0\rangle_{0,n} |\Phi\rangle_{1\ldots N\neq n}, \tag{2.5}$$

subject to the normalization condition

$$\left(\sum_{n=1}^{N} \beta_n\right)^2 + (d-1)\sum_{n=1}^{N} \beta_n^2 = d. \tag{2.6}$$

The state $|\Phi\rangle$ is the (normalized) uniform superposition over all permutations of $|B_0\rangle^{\otimes(N-1)/2}$ for odd N, and $|B_0\rangle^{\otimes(N-2)/2}|0\rangle$ for even N. Each covering satisfies

$$(|B_0\rangle\langle B_0|_{0,m} \otimes \mathbb{1}) |B_0\rangle_{0,n} |\Phi\rangle = \gamma_{n,m} |B_0\rangle_{0,m} |\Phi\rangle,$$

where

$$\gamma_{n,m} = \left(\tfrac{1}{d} + \delta_{n,m}\left(1 - \tfrac{1}{d}\right)\right),$$

which means that $|\Psi\rangle$ is an eigenstate of R provided

$$\alpha_n d \sum_{m=1}^{N} \gamma_{n,m}\beta_m = (d(d+1)\lambda - 1)\beta_n \qquad \forall n.$$

Thus, to relate the $\{\alpha_n\}$ to the $\{\beta_n\}$, one just has to find the maximum eigenvector of an $N \times N$ matrix $\sum_{n,m} \alpha_n \gamma_{n,m} |n\rangle\langle m|$. This does not prove that it is the *maximum* eigenvector of R that we are looking for. Let us, however, proceed under that assumption. The singlet fractions of $|\Psi\rangle$ are

$$p_{0,n} = \left(\sum_{m=1}^{N} \gamma_{n,m}\beta_m\right)^2.$$

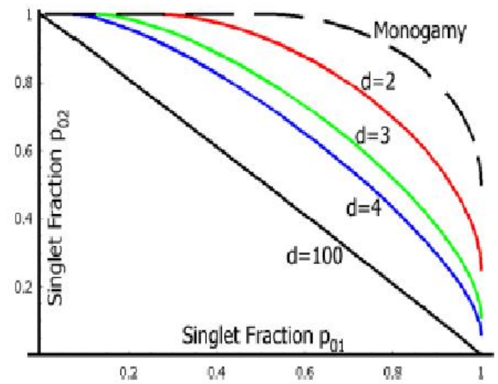

Figure 2.2: For a 3-qudit state maximally entangled between spin 0 and spins 1,2, the optimal trade-off between singlet fractions derived from the tangle monogamy (dashed line, qubits only) and singlet monogamy ($d = 2, 3, 4, 100$).

After some rearrangement, the $\{\beta_n\}$ can be eliminated by substituting for $\{p_{0,n}\}$ in Eq. (2.6), yielding the equality of the following 'singlet monogamy' relation for the singlet fractions of the cloners,

$$\sum_{n=1}^{N} p_{0,n} \leq \frac{d-1}{d} + \frac{1}{N+d-1}\left(\sum_{n=1}^{N}\sqrt{p_{0,n}}\right)^2. \tag{2.7}$$

The above relation encapsulates the optimal trade-off in fidelities (expressed here in terms of the singlet fractions) for the universal $1 \to N$ asymmetric qudit cloning problem. The inequality can be derived by assuming equality and replacing $p_{0,n}$ with $p_{0,n} + \varepsilon_n$. The special case of $1 \to 2$ cloning is depicted in Fig. (2.2).

We are now in a position to compare Eqn. (2.7) to previous results. Setting all the $p_{0,n}$ equal returns the known result for universal symmetric cloning [16] of

$$F = \frac{1}{N} + \frac{2(N-1)}{N(d+1)}.$$

Similarly, the $1 \to 1+1+1$ and $1 \to 1+N$ qubit cloners [37] can be found. The latter case was parametrized as $F_1 = 1-2y^2/3, F_N = \frac{1}{2}+\frac{1}{3N}(y^2+\sqrt{N(N+2)}xy)$, where $x^2+y^2 = 1$. Our solution is consistent with this, where $y^2 = N(N+2)\beta_N^2/4$ and $x = \beta_1 + \frac{1}{2}N\beta_N$. Thus, we know that at least at certain points of the phase diagram, $|\Psi\rangle$ is the maximum eigenvector of R which indicates that the ansatz state may well be the universal cloner that we are looking for. This has also been confirmed analytically for $d = 2, N \leq 5$ and $d \leq 5, N = 3$ for all asymmetries. A detailed proof based on the Lieb-Mattis theorem showing analytically that $|\Psi\rangle$ is indeed the maximum eigenvector of R has also recently been found in [24].

2.4 Applications of Singlet Monogamy

While the phenomenon of entanglement monogamy is well-known, a quantitative relationship has only been derived for the case of the entanglement measure, τ, for qubits called the tangle [26, 27]. The tangle for qubits is simply the square of the concurrence $C(\rho)$ defined as $C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$ [28] in which λ_k are the eigenvalues of the Hermitian matrix $\sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$ listed in decreasing order. $\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$ is the spin flipped state of ρ, and σ_y is a Pauli matrix. For mixed states, the concurrence is defined by convex roof extension. The monogamy relation for the tangle states that the tangle of a qubit with the rest of the system cannot be smaller than the sum of the tangles of qubit pairs which it is part of, as per the inequality

$$\sum_{n=1}^{N} \tau(\rho_{0,n}) \leq \tau(\rho_{0,1\ldots N}). \tag{2.8}$$

The use of this entanglement monogamy relation in the calculation of the ground state and thermal state properties of certain Hamiltonians has also been demonstrated. However, there are many situations where singlet fraction is a more relevant parameter to estimate than the tangle, and thus no-cloning bounds give much tighter results. Consider, for example, the Heisenberg model on a regular lattice of coordination number c and N spins.

$$H_{\text{Heis}} = \tfrac{1}{4}\sum_{\langle i,j\rangle}(XX + YY + ZZ)_{i,j},$$

for which we might like to bound the ground state energy. The ground state can be taken to be $|\Psi\rangle$, with energy per site $E = \langle\Psi| H_{\text{Heis}} |\Psi\rangle / N$. However, this can be rephrased as simply the sum of singlet fractions of $|\Psi\rangle$ for all nearest-neighbor pairs,

$$EN = \tfrac{1}{8}Nc - \sum_{\langle i,j\rangle} p_{i,j}.$$

The ground state must reproduce the translational invariance of the Hamiltonian, so all the singlet fractions are equal, $E = \frac{1}{2}c(1/4 - p)$. By assuming the tangle monogamy, the tangle possible between a pair of neighboring sites is $\tau \leq 1/c$, which yields $p \leq \frac{1}{2}(1+1/\sqrt{c})$. By contrast, the singlet monogamy relation for qubits reveals that $p \leq \frac{1}{2}(1 + 1/c)$, giving a much tighter bound for E. This same bound has previously been achieved in [38], which used the technique of dividing the lattice into small repeating units, and diagonalizing the corresponding Hamiltonian [31] – the sum of ground state energies of blocks of terms is a lower bound to the overall ground state energy. Differing coupling strengths along different spatial directions can be accounted for using asymmetric cloning, and performing an optimization over the asymmetry parameters.

Extending this [27] serves to demonstrate a feature of our formulation of singlet monogamy; spin 0 is taken to be maximally entangled with the other spins. In comparison, the monogamy relation of Eqn. (2.8) allows an arbitrary value for $\tau(\rho_{0,1\ldots N})$, although it is often hard to determine, and commonly set to its maximal value of 1 for qubits. For a translationally invariant spin-$\frac{1}{2}$ system with magnetization $\langle S_{\vec{n}}\rangle$ along direction $\vec{n}$, the tangle $\tau(\rho_{0,1\ldots c}) \leq (1-\langle S_{\vec{n}}\rangle^2)^2$ [27], which can be used to impose a bound on the singlet fraction, and thus the validity of a mean-field approximation of the energy of a Heisenberg Hamiltonian,

$$\varepsilon \leq p_{0,1} - \tfrac{1}{2} \leq (1-\langle S_{\vec{n}}\rangle^2)/\sqrt{4c}.$$

Crucially, as the coordination number increases, the accuracy, ε, of the mean-field approximation improves. Although singlet monogamy has no way to incorporate the bound on τ, we still arrive at

$$\varepsilon \leq p_{0,1} - \tfrac{1}{2} \leq 1/(2c),$$

which is a better bound for $\langle S_{\vec{n}}\rangle^2 \leq 1 - 1/\sqrt{c}$, proving that the mean-field approximation converges even faster with increasing coordination number. Potentially, one could choose a telecloning state $|\Psi\rangle$ such that $tr(R\,|\Psi\rangle\langle\Psi|)$ is maximum under the constraint that $|\Psi\rangle$ has some specific entanglement, which would serve to relax this property. This is left open for future study.

2.5 State Dependent $1 \to N$ Qubit Cloning

Having studied the universal $1 \to N$ cloning of qudits, we now turn to apply the formalism using the Jamiolkowski isomorphism to the more common case of qubits ($d = 2$) where the input state is now restricted to a particular distribution $f(\psi)$. The general form of the qubit input state is given as

$$|\psi\rangle = \cos\frac{\theta}{2}\,|0\rangle + \sin\frac{\theta}{2}e^{i\phi}\,|1\rangle$$

with an as yet unspecified distribution function $f(\theta, \phi)$.

We now develop a parametrization of the $1 \to N$ asymmetric cloning of qubits for a large class of state dependent cloners, including equatorial and universal cloners. To do this, we impose two restrictions on the input distribution function $f(\theta, \phi)$, namely: (i) This distribution function $f(\theta, \phi)$ is phase covariant, meaning it is independent of ϕ, i.e., $f(\theta, \phi) = f(\theta)$ and (ii) The distribution is symmetric about the equator of the Bloch sphere, i.e., $f(\theta) = f(\pi - \theta)$. These assumptions allow us to make a smooth transition from equatorial to universal cloning by picking as the input state distribution segments of increasing size about the equator of the Bloch sphere.

Using these assumptions, the matrix R in Eq.(2.3) for the $1 \to N$ cloning of qubits can be written as

$$R = \tfrac{1}{2}\mathbb{1} + \sum_{n=1}^{N} \alpha_n \Gamma \left(XX - YY + \frac{1-4\Gamma}{2\Gamma} ZZ \right)_{0,n},$$

where

$$\Gamma = \frac{1}{4} \int f(\theta,\phi) \sin^2\theta d\theta d\phi.$$

The parameter, Γ, varying between 0 and $\frac{1}{4}$ provides an intuitive interpretation regarding the distribution of states over the Bloch sphere - the larger the value, the more tightly packed the states are around the equator. When the parameter Γ is 0, we are restricted to the classical states $|0\rangle$ and $|1\rangle$ for which we expect perfect copying. The case $\Gamma = \frac{1}{6}$ recovers the universal cloning problem discussed in the previous sections. When $\Gamma = \frac{1}{4}$, we obtain the case of equatorial cloning, where the input qubit is restricted to lie on the equator of the Bloch sphere.

We would now like to find the maximum eigenvector and maximum eigenvalue of the above matrix R. The problem can be recast by applying a rotation Y_0 to R, and instead demanding the minimum eigenvector (ground state) of a new matrix $\tilde{R}$ given as

$$\tilde{R} = -\tfrac{1}{2}\mathbb{1} + \sum_{n=1}^{N} \alpha_n \Gamma \left(XX + YY + \frac{1-4\Gamma}{2\Gamma} ZZ \right)_{0,n}.$$

This matrix $\tilde{R}$ is familiar as the Hamiltonian for an anisotropic Heisenberg model on a star configuration. We now proceed to calculate the optimal fidelities in case of symmetric cloning, where each of the outputs is required to have the same quality of clone.

2.5.1 Symmetric Cloning

The most commonly studied instance of cloning is where all the output copies are required to have the same fidelity, so $\alpha_n = \frac{1}{N}$. Thus, we have

$$\begin{aligned} \tilde{R} = -\tfrac{1}{2}\mathbb{1} \quad &+ \quad \Gamma \left(X_I \left(\frac{1}{N} \sum_{n=1}^{N} X_n \right) + Y_I \left(\frac{1}{N} \sum_{n=1}^{N} Y_n \right) \right) \\ &+ \quad \frac{1-4\Gamma}{2} \left(Z_I \left(\frac{1}{N} \sum_{n=1}^{N} Z \right) \right), \end{aligned}$$

The permutation invariance on the qubits $1 \dots N$ mean that the operators in the above expression such as $\left(\frac{1}{N} \sum_{n=1}^{N} X_n \right)$ reduce into a simple direct sum structure. In the present instance, it is known that for the Heisenberg model, the minimal eigenvalue that we require will always be taken from the fully symmetric subspace [39]. The maximum fidelity that can be realized in the cloning transformation is thus given by

$$F = \tfrac{1}{2} + \frac{1-4\Gamma}{2N} + \frac{1}{N} \max_{i=0\ldots N-1} \sqrt{4\Gamma^2(i+1)(N-i) + (\tfrac{1}{2}-2\Gamma)^2(N-2i-1)^2}.$$

The choice of the best i in the maximization above depends on the value of Γ. Treating the term to be maximized as a continuous function of i, one can maximize it in the standard manner, finding that for $\frac{1}{6} \leq \Gamma \leq \frac{1}{4}$, the i should ideally be $(N-1)/2$. However, since i must be an integer, it takes the value $\lfloor N/2 \rfloor$. We therefore find that for this regime of Γ (between $\frac{1}{6}$ and $\frac{1}{4}$), the fidelity is given by

$$F = \begin{cases} \frac{1}{2} + \frac{1}{2N} + \frac{\Gamma}{N}(N-1) & N \text{ odd} \\ \frac{1}{2} + \frac{1-4\Gamma}{2N} + \frac{1}{N}\sqrt{\Gamma^2 N(N+2) + (\frac{1}{2}-2\Gamma)^2} & N \text{ even} \end{cases}$$

Outside of that range of Γ, for $0 \leq \Gamma \leq \frac{1}{6}$, the term is maximized when i is either 0 or $N-1$ (both give the same fidelity). The fidelity in this parameter regime is then given by

$$F = \tfrac{1}{2} + \frac{1-4\Gamma}{2N} + \frac{1}{N}\sqrt{4N\Gamma^2 + (N-1)^2(\tfrac{1}{2}-2\Gamma)^2}.$$

We now analyze the above results for the fidelities comparing them to the known cases of classical states, universal cloning and equatorial cloning.

Classical States

If the subset of possible states is only $|0\rangle$ or $|1\rangle$, then it is clear that one should be able to achieve the maximum cloning fidelity $F = 1$, this being simply classical copying. This is indeed the case, because when $\Gamma = 0$ for the classical states, the maximum eigenstates of R are $|0\rangle^{\otimes(N+1)}$ and $|1\rangle^{\otimes(N+1)}$. Moreover, one can construct a maximum eigenvector that is maximally entangled given by

$$\frac{1}{\sqrt{2}}\left(|0\rangle^{\otimes(N+1)} + |1\rangle^{\otimes(N+1)}\right),$$

proving that there exists a unitary that achieves the optimal fidelity of cloning (the cloning is therefore economic).

Universal Cloning

In the case of universal cloning, the state $|\psi\rangle$ is selected uniformly over the surface of the Bloch sphere, $\Gamma = \frac{1}{6}$, and R becomes the Hamiltonian of the isotropic Heisenberg model. As described in previous sections, we recover the optimal fidelity of symmetric universal cloning given by [16]

$$F = \frac{2N+1}{3N}.$$

Equatorial Cloning

In the case of equatorial cloning, we restrict the set of states to the input distribution function $f(\theta)$ with the specific choice of $\theta = \pi/2$. In this situation, we clone states that are on the equator of the Bloch sphere and $\Gamma = \frac{1}{4}$. The fidelity of the cloning for the fully symmetric case [40] is now recovered by our previous considerations as

$$F = \begin{cases} \frac{3N+1}{4} & N \text{ odd} \\ \frac{1}{2} + \frac{\sqrt{N(N+2)}}{4N} & N \text{ even} \end{cases}$$

Monogamy of Bell inequalities:

Before concluding our analysis of $1 \to N$ qubit cloning, we now turn to prove how the monogamy relation of the Clauser-Horne-Shimony-Holt (CHSH) Bell inequality [41] arises from the consideration of $1 \to 2$ asymmetric equatorial cloning. The CHSH inequality is explained in detail in the next chapter, here we only use the fact that the general CHSH operator between two entangled qubits at sites 0 and n can be written in quantum theory as

$$\mathcal{B}_{0n} = \sqrt{2}(XX - YY)_{0n},$$

up to local unitaries. The above form arises due to the fact that up to local unitaries, the individual settings in the Bell inequality can be chosen to lie in the X-Y plane by both parties. Moreover, for optimal violation for any quantum state, the local settings should be chosen such that they are as far away from being commuting as possible [42]. In this scenario, we would like to derive the optimal trade-off between the CHSH inequality violation between two parties Alice and Bob (each holding a qubit state) and the violation of the CHSH inequality by Alice and another party Charlie, i.e., between $\mathcal{B}_{01}$ and $\mathcal{B}_{02}$. We now recall that in the asymmetric equatorial qubit cloning problem, maximizing the cloning fidelity corresponds to finding the maximum eigenvalue, λ, of

$$R = \tfrac{1}{2}\mathbb{1} + \frac{1}{4\sqrt{2}}\left(\alpha_1\mathcal{B}_{01} + \alpha_2\mathcal{B}_{02}\right).$$

This implies that the average values of the two CHSH parameters for any state, $\langle\mathcal{B}_{01}\rangle$ and $\langle\mathcal{B}_{02}\rangle$, obey the inequality

$$\alpha_1\langle\mathcal{B}_{01}\rangle + \alpha_2\langle\mathcal{B}_{02}\rangle \le 4\sqrt{2}(\lambda - \tfrac{1}{2})$$

where the maximum eigenvalue is given by $\lambda = \frac{1}{2}(\sqrt{\alpha_1^2 + \alpha_2^2} + 1)$. The two asymmetry parameters α_1 and α_2 are required to obey the condition $\alpha_1 + \alpha_2 = 1$, so we can choose them to obey

$$\alpha_1 = \langle\mathcal{B}_{01}\rangle\kappa \qquad \alpha_2 = \langle\mathcal{B}_{02}\rangle\kappa,$$

with a parameter κ chosen to satisfy the normalization condition. Setting these choices for the asymmetry parameters in the inequality, we derive the well-known monogamy relation for the Bell-CHSH inequality within quantum theory [45]

$$\langle \mathcal{B}_{01} \rangle^2 + \langle \mathcal{B}_{02} \rangle^2 \leq 8.$$

This procedure can be followed to derive monogamy relations in other scenarios as well, the case of equatorial qubit cloning always corresponding to a monogamy relation for the CHSH inequalities. This is due to the fact that these Bell inequalities involve two settings for each observer which can be chosen to lie on the equator of the local Bloch spheres, and this results in exactly the same form of optimization problem as in the $1 \to N$ equatorial qubit cloning problem. In fact, the violation of the CHSH inequality by a two qubit state may be directly related to the equatorial cloning fidelity using that state just as the cloning fidelity for universal cloning is related to the singlet fraction of the state. For larger values of N however, the maximum eigenvalue λ is not straightforward to derive for general asymmetries.

2.6 Conclusions and Open Questions

The formalism using the Jamiolkowski isomorphism has been utilized here to identify the solution to the most interesting cloning problem, namely the $1 \to N$ asymmetric universal qudit cloning. From the solution written as a trade-off in the optimal fidelities, a monogamy relation for entanglement in terms of singlet fraction was derived. Applications of the monogamy relation in condensed matter scenarios were demonstrated.

The question of economic implementation of the cloner needs to be addressed. A generalization of the considered situation is the $M \to N$ universal cloning where in place of a single copy, we have M copies of the input state to be cloned. A solution to this problem in the case of symmetric cloning is known, while the general asymmetric case remains hard to solve. The formalism presented here, and, primarily, the techniques for proving optimality, can potentially be applied in many other scenarios. A natural generalization involves the cloning of mixed quantum states, a problem known as broadcasting [46] and cloning for continuous variable systems [47]. It is also potentially interesting to consider the optimal cloning of specific properties such as entanglement rather than entire quantum states [48].

Finally, with regard to state-dependent cloners, we have investigated a wide variety of state dependent cloners for qubits including equatorial and universal cloning, finding solutions in the symmetric case, the general asymmetric situation still remaining unsolved. For the specific case of $1 \to 2$ equatorial cloning, we found that the trade-off in the achievable fidelities leads to the monogamy relation for the well-known CHSH Bell inequalities. In the next chapter, we turn to a more detailed study of the phenomenon of monogamy in Bell inequality violations and find other principles from which these can be derived.

Chapter 3

Monogamy of Bell Inequality Violations

Violation of a Bell inequality is one of the defining tests of the "quantumness" of a system distinguishing it from all classical systems (that conform to the idea of local realism). The violations of Bell inequalities by microscopic systems such as a system of two qubits have been clearly observed in experiments. While not all the possible loopholes have been simultaneously closed yet, most physicists agree that a local realistic description of most entangled microscopic systems is untenable. In the typical Bell experiment, a composite (quantum entangled) system is split between many parties who then proceed to perform measurements on their respective subsystems. After recording their outcomes, they meet at the end of the experiment to calculate the correlations of their measurement results and check whether they have succeeded in obtaining a violation of local realism, i.e., whether the measurement outcomes when plugged in a Bell parameter violate its local realistic bound. In this chapter, we study the violations of the correlation Bell inequalities, concentrating on an intriguing feature of these, namely their monogamy relations.

3.1 The Bell-CHSH inequality

We begin with a brief explanation of the most well-known Bell inequality, that due to Clauser, Horne, Shimony and Holt, the Bell-CHSH inequality [41]. Bell's inequality is not a result about quantum mechanics so our considerations will initially involve only the "common sense" notions introduced by EPR and expected of a physical theory. After formulating the Bell inequality based on these notions, we will see how the correlations in many entangled quantum states violate the inequality showing that Nature does not conform to this common sense world view.

The experiment begins with a source preparing two particles (in a repeatable manner) and sending one particle each to the two experimentalists Alice and Bob who are in spatially separate locations (see Fig. 3.1). Alice and Bob are each in possession of two local measurement apparatuses (or two measurement settings with the same apparatus) which we denote by A_1, A_2 and B_1, B_2 respectively. With absolute freedom, Alice and Bob choose one of their apparatus and perform a local measurement on their respective particle. In this manner, in each experimental run (where they receive a particle from the source) they obtain measurement outcomes, a_1, a_2 and b_1, b_2 respectively, each of which are taken to be dichotomic, i.e. each measurement has two outcomes which are assigned the value $+1$ or -1. The free-will assumption alluded to refers to the fact that Alice and Bob themselves need not know in advance which measurement (A_1 or A_2, alternatively B_1 or B_2) they will choose to perform, the measurement settings are chosen in a random manner. We now make the assumption of "realism", namely that $A_{1(2)} = a_{1(2)}$ (similarly for Bob) is an objective realistic property of Alice's (Bob's) particle which is merely revealed by the measurement. In other words, the outcomes of measurements exist prior to and independent of the act of measurement. The second assumption we make in deriving the Bell inequality is that of "locality". Locality assumes that the outcomes of Alice (and Bob) depends on her (his) local measurement setting alone, and are independent of the setting chosen by the other party. In order to implement this locality in our experiment, we demand that the Alice and Bob do their measurements simultaneously (or at least in a causally disconnected manner) so that there is no possibility of Alice's measurement setting influencing the result of Bob's measurement (and vice versa). Recall that physical influences cannot propagate faster than light, as necessitated by the theory of relativity.

We now arrive at the following algebraic identity for the outcomes in every experimental run:

$$a_1(b_1 + b_2) + a_2(b_1 - b_2) = \pm 2.$$

This identity follows from the fact that $a_1, a_2 = \pm 1$ and $b_1, b_2 = \pm 1$ so that either $b_1 + b_2 = 0$ and $b_1 - b_2 = \pm 2$ or $b_1 + b_2 = \pm 2$ and $b_1 - b_2 = 0$. After averaging over many experimental runs, one obtains the expression

$$-2 \leq \langle A_1 B_1 \rangle + \langle A_1 B_2 \rangle + \langle A_2 B_1 \rangle - \langle A_2 B_2 \rangle \leq 2.$$

These bounds arise due to the fact that one cannot exceed the extremal values of the expression by averaging. This implies that even if the outcomes for each A_j and B_k ($j, k \in \{1, 2\}$)are probabilistic, the average value of the above CHSH expression is bounded by ± 2 for all local realistic theories. In other words, we can define the local realistic correlation function for the outcomes of measurements A_j and B_k ($j, k = 1, 2$) as

$$E(A_j, B_k)_{LR} = \sum_{a_1, a_2, b_1, b_2} p(A_1 = a_1, A_2 = a_2, B_1 = b_1, B_2 = b_2) a_j b_k.$$

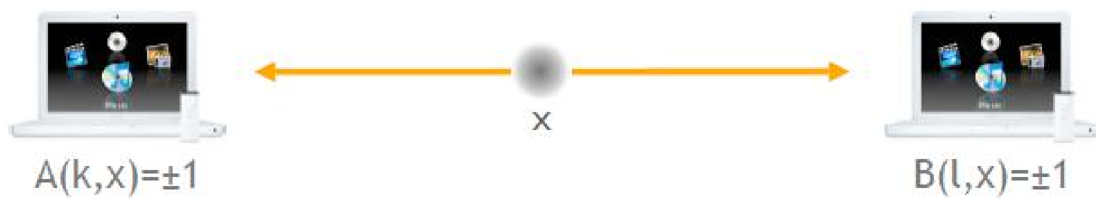

Figure 3.1: The experimental scenario where a source sends a particle each to spatially separated Alice and Bob. They each choose one of two local measurement settings, their choice denoted by k and l, and obtain the dichotomic outcomes $+1$ or -1. Therefore, for each run x, we have that $A(1,x)[B(1,x)+B(2,x)]+A(2,x)[B(1,x)-B(2,x)]=\pm 2$.

and we arrive at the Bell-CHSH inequality

$$\Big|E(A_1,B_1)_{LR}+E(A_1,B_2)_{LR}+E(A_2,B_1)_{LR}-E(A_2,B_2)_{LR}\Big|\leq 2. \tag{3.1}$$

Here the joint probability for the outcomes of all the measurements $p(A_1=a_1,A_2=a_2,B_1=b_1,B_2=b_2)$ exists by virtue of the (local) realistic assumption [49]. In fact, the existence of the joint probability distribution is the defining feature of all (local) realistic theories and characterizes a polytope of correlations that fall within the local realistic category. As we shall see, quantum mechanical correlations can fall outside this domain giving rise to the violation of Bell inequalities. We note that the CHSH inequality for two parties and two measurement settings per party is part of a larger set of inequalities that are generically known as Bell inequalities. Indeed, a number of such inequalities involving multiple parties and multiple measurement settings for each party are known [50].

We now show that the correlations in some entangled quantum states can violate the Bell-CHSH inequality. We take the archetypal example of Alice and Bob holding one particle each of the singlet state of two spin-1/2 particles (qubits),

$$|\psi_-\rangle=\frac{1}{\sqrt{2}}(|01\rangle-|10\rangle).$$

Here the state $|0\rangle$ (respectively $|1\rangle$) refers to the spin pointing up (respectively down) along the local z direction (this choice is arbitrary) for each of the two qubits. For this state, the quantum mechanical correlation function reads

$$E(A_j,B_k)_{QM}=tr[|\psi_-\rangle\langle\psi_-|(\vec{a}_j\cdot\vec{\sigma}\otimes\vec{b}_k\cdot\vec{\sigma})]=-\vec{a}_j\cdot\vec{b}_k,$$

where $\vec{a}_j\cdot\vec{b}_k$ refers to the scalar product of the two vectors $\vec{a}_j$ and $\vec{b}_k$ which denote the local measurement directions of Alice and Bob. The local measurements are $\vec{a}_j\cdot\vec{\sigma}$ and $\vec{b}_k\cdot\vec{\sigma}$, where $\vec{\sigma}$ refers to the vector $\{\sigma_x,\sigma_y,\sigma_z\}$ of Pauli matrices. Thus quantum mechanics predicts for the left-hand side of (3.1)

$$B_{CHSH}^{QM} = \left| \vec{a}_1 \cdot (\vec{b}_1 + \vec{b}_2) + \vec{a}_2 \cdot (\vec{b}_1 - \vec{b}_2) \right|.$$

In order to find the maximum value of this expression, one can introduce normalized orthogonal vectors $\vec{b}_+$ and $\vec{b}_-$ such that:

$$\begin{aligned} \vec{b}_1 + \vec{b}_2 &= 2\cos\alpha\ \vec{b}_+, \\ \vec{b}_1 - \vec{b}_2 &= 2\sin\alpha\ \vec{b}_-. \end{aligned}$$

The expression then transforms to

$$B_{CHSH}^{QM} = \left| 2\cos\alpha\ \vec{a}_1 \cdot \vec{b}_+ + 2\sin\alpha\ \vec{a}_2 \cdot \vec{b}_- \right|.$$

The maximum value is attained by the choice $\vec{a}_1 = \vec{b}_+$, $\vec{a}_2 = \vec{b}_-$ and $\alpha = \frac{\pi}{4}$ giving the maximal quantum value as

$$B_{CHSH}^{QM}(max) = 2\sqrt{2},$$

which is above the local realistic bound of 2. In other words, the maximal value is attained when the measurement vectors for Alice and Bob lie in the same plane, the measurements for the singlet state being given by

$$\begin{aligned} &A_1 = \sigma_z, A_2 = \sigma_x \\ &B_1 = \frac{-\sigma_z - \sigma_x}{\sqrt{2}}, B_2 = \frac{\sigma_z - \sigma_x}{\sqrt{2}}. \end{aligned}$$

This maximal value of $2\sqrt{2}$ is known as the Tsirelson bound [42], being the maximum value of the Bell-CHSH expression within quantum theory, the maximal violation then being $2\sqrt{2} - 2$. Violation of this Bell inequality has been confirmed in numerous experiments, e.g. [51, 52, 53, 54]. For all pure entangled two-qubit states, one can find measurements that lead to a violation of the Bell-CHSH inequalities. This ceases to be true for mixed states however, with the famous example [55] of the so-called Werner states that in a certain parameter regime do not violate any Bell inequality in spite of being entangled.

3.2 Monogamy of Bell inequality violations

An interesting phenomenon occurs when a single party is involved in more than one Bell experiment, i.e. when the measurement results of one party are plugged into more than one Bell parameter. Trade-offs exist between the strengths of violations of Bell inequalities, and in many cases the violation of a Bell inequality with one party precludes the violation with any other party. This phenomenon is known as the “monogamy of

Bell inequality violations" and is the focus of the present chapter. The first theorems establishing monogamy relations were given in [43, 44, 45] and are stated in terms of the Bell-CHSH parameter B_{AB} (involving two observables per party)

$$B_{AB} = A_1 \otimes (B_1 + B_2) + A_2 \otimes (B_1 - B_2).$$

The CHSH monogamy relation: Suppose that three parties, A, B, and C, share a quantum state (of arbitrary dimension) and each chooses to measure one of two observables. Then, the quantum values of the Bell-CHSH parameters B_{AB} and B_{AC} for any state obey

$$\langle B_{AB}\rangle^2 + \langle B_{AC}\rangle^2 \leq 8. \tag{3.2}$$

Noting that the local realistic bound in the CHSH inequality is 2, one sees immediately from the above inequality that when $B_{AB} \geq 2$, $B_{AC} \leq 2$ and vice versa. This is precisely the notion of monogamy; when Alice and Bob obtain a violation of the Bell inequality, Alice and Charlie are unable to do so and vice versa. As we have seen above, the maximum value (Tsirelson bound) of a single CHSH parameter within quantum theory is given by $B_{AB} = 2\sqrt{2}$, this then implies that $B_{AC} = 0$ meaning that if one Bell inequality is maximally violated, the other Bell parameter acquires value 0. This supports the notion from entanglement monogamy that when a spin is maximally entangled with another spin (so that the reduced density matrix of each spin is the identity), its entanglement with any other spin vanishes. In fact, the Tsirelson bound of $2\sqrt{2}$ can be obtained as a corollary to the above CHSH monogamy relation in precisely the above manner, setting $B_{AC} = 0$ recovers $B_{AB} = 2\sqrt{2}$. Bell monogamies have been shown to be useful in showing security for some key distribution protocols [56], in interactive proof systems [44], and as we shall see in the subsequent chapter, they are at the heart of the emergence of a local realistic description for correlations in macroscopic systems.

Within all theories that obey the so called no-signaling principle, a weaker monogamy was also established [44],

$$|\langle B_{AB}^{NS}\rangle| + |\langle B_{AC}^{NS}\rangle| \leq 4.$$

Quantum theory itself obeys the no-signaling principle and therefore the above relation also holds within the theory. However, this linear monogamy relation is clearly weaker than the quadratic monogamy relation within quantum theory established in Eq. (3.2) showing that no-signaling does not completely capture the monogamy of Bell inequalities in the quantum scenario.

That Bell monogamy relations (BMR) arise within all no-signaling theories was first observed in [57] and an instructive method to derive these was shown in [58]. We firstly state and refine this method as a precursor to its generalization to the phenomenon of "monogamy of contextuality" in a later chapter. Bell monogamies also arise within quantum theory such as in Eq. (3.2). Within this theory, we show that they can be derived as a consequence of the "correlation complementarity" principle in the next section. Methods to derive Bell monogamies within quantum theory using this principle are then developed using graph-theoretic techniques. The material in this chapter covers but is not restricted to [59], and includes new results concerning multipartite monogamies in all no-signaling theories and general bipartite monogamies within quantum theory.

3.3 Bell monogamies in all no-signaling theories

The no-signaling principle can be understood as the statement that no signal can be transmitted instantaneously (or even faster than a finite maximum speed such as the speed of light) and therefore probabilities of measurement outcomes are independent of measurement settings at spatially separated locations. It is mathematically stated as the following constraint on probabilities of measurement outcomes

$$P(a|A,B) = P(a|A).$$

Here A and B are the measurement settings used by two spatially separated parties Alice and Bob, and a denotes the outcome of Alice's measurement A. The principle therefore states that the probability of obtaining an outcome a upon measuring observable A is independent of the measurement setting B chosen at a spatially separated location.

In this section, we will explain (and refine) the method introduced in [58] for the derivation of Bell monogamy relations within all no-signaling theories. The technique introduced here will also be useful for the derivation of monogamy relations in contextuality in a later chapter. We begin with a general linear bipartite (between two parties, Alice and Bob) Bell inequality for correlations which has the form

$$B(A,B) = \sum_{x,y,a,b} \alpha(x,y,a,b) P(A_x = a, B_y = b) \leq R.$$

Here x and y enumerate the local measurement settings (A and B) of Alice and Bob respectively while a and b denote their measurement outcomes. We do not restrict ourselves to dichotomic (two outcome) measurements here and therefore the derived monogamies will apply in the quantum case to systems of arbitrary local Hilbert space dimension. Here, R denotes the local realistic bound of the inequality while $P(A_x = a, B_y = b)$ denotes the probability that Alice obtains outcome a when she chooses to measure A_x and Bob obtains outcome b when he chooses the measurement setting B_y. Any bipartite linear Bell inequality can be written in this form and by suitable maneuvering one can choose the coefficients $\alpha(x,y,a,b) \geq 0$ and $R \geq 0$. For instance, if a particular $P(\tilde{A}_x = \tilde{a}, \tilde{B}_y = \tilde{b})$ appears with a negative coefficient, by writing this probability as 1 minus the probability of all the complementary events and shifting all constant terms to the right, we can ensure that the terms on the left hand side of the inequality appear with positive coefficients.

We consider the scenario in which Alice tries to violate the same Bell inequality $B(A, B^m)$ with each of a set of n Bobs $\{B^1, \ldots, B^n\}$, i.e. $m = 1, \ldots, n$. Under the constraint that the number of measurement settings for each Bob (B^m) is less than or equal to the number of Bobs n (note that the number of measurement settings for Alice is unrestricted), it was shown that the following monogamy relation holds in any no-signaling theory

$$\sum_{m=1}^{n} B(A, B^m) \leq nR.$$

Here we present an alternative graph-theoretic proof of the above statement than the original proof in [58]. For simplicity, we explain the proof for the basic scenario in which Alice tries to violate the Bell-CHSH inequality with Bob and Charlie. The proof technique can easily be extended to the general scenario explained above as well. Consider the violation of a Bell-CHSH inequality involving two measurement settings for each of two spatially separated systems labeled Alice and Bob, and also for the two separated systems Alice and Charlie. As before, denote the measurements performed by Alice as A_1 and A_2, those by Bob as B_1 and B_2 and those by Charlie as C_1 and C_2. The spatial separation guarantees that any set of measurements A_i, B_j, C_k can be jointly performed and that measurement pairs $\{A_1, A_2\}$, $\{B_1, B_2\}$ and $\{C_1, C_2\}$ are not jointly measurable in general. One can depict this situation in graph-theoretic notation using a "commutation graph" as in Fig. 3.2. The vertices of this graph denote the different measurements while edges join two vertices if the corresponding measurements can be jointly performed. The two CHSH inequalities with local realistic bounds R (= 2) are expressed as

$$B(A_1, A_2, B_1, B_2) = \langle A_1 \otimes B_1 \rangle + \langle A_1 \otimes B_2 \rangle + \langle A_2 \otimes B_1 \rangle - \langle A_2 \otimes B_2 \rangle \leq R$$

and similarly for Alice and Charlie,

$$B(A_1, A_2, C_1, C_2) = \langle A_1 \otimes C_1 \rangle + \langle A_1 \otimes C_2 \rangle + \langle A_2 \otimes C_1 \rangle - \langle A_2 \otimes C_2 \rangle \leq R.$$

Here $\langle A_k \otimes B_k \rangle$ denotes the average of the enclosed quantity. The monogamy relation for these two inequalities can be derived using no-signaling in this graph-theoretic formalism as follows.

We first note that the commutation graph Fig. (3.2) can be vertex decomposed into two sub-graphs of four vertices, each of which represents a single Bell inequality, namely the sub-graphs A_1, A_2, B_1, C_2 and A_1, A_2, B_2, C_1 where we ignore edges in the original graph connecting the two resulting sub-graphs. In other words, the expression $B(A_1, A_2, B_1, B_2) + B(A_1, A_2, C_1, C_2)$ can be exactly rewritten as the sum of two different

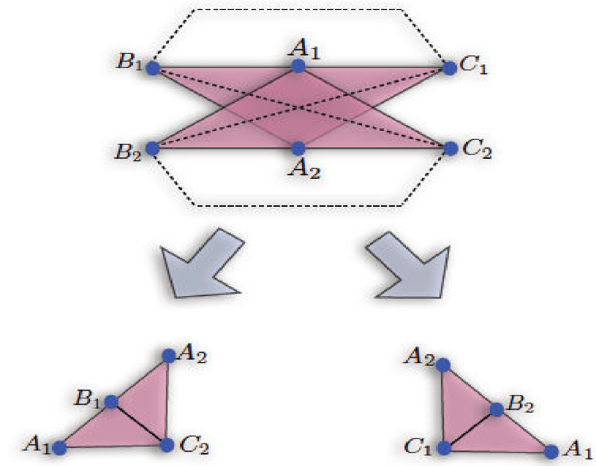

Figure 3.2: The commutation graph (top) and its decomposition (bottom) leading to the Bell-CHSH monogamy relation in no-signaling theories.

Bell expressions as $B(A_1, A_2, B_1, C_2) + B(A_1, A_2, C_1, B_2)$. Here

$$B(A_1, A_2, B_1, C_2) = \langle A_1 \otimes B_1 \rangle + \langle A_1 \otimes C_2 \rangle + \langle A_2 \otimes C_1 \rangle - \langle A_2 \otimes C_2 \rangle$$

and

$$B(A_1, A_2, C_1, B_2) = \langle A_1 \otimes C_1 \rangle + \langle A_1 \otimes B_2 \rangle + \langle A_2 \otimes C_1 \rangle - \langle A_2 \otimes B_2 \rangle .$$

The idea behind this vertex decomposition is that a joint probability distribution reproducing all measurable marginals can be constructed for each of the Bell expressions $B(A_1, A_2, B_1, C_2)$ and $B(A_1, A_2, C_1, B_2)$. For instance for the sub-graph A_1, A_2, B_1, C_2 we can construct

$$p(A_1 = a_1, A_2 = a_2, B_1 = b_1, C_2 = c_2) = \frac{p(A_1 = a_1, B_1 = b_1, C_2 = c_2)p(A_2 = a_2, B_1 = b_1, C_2 = c_2)}{p(B_1 = b_1, C_2 = c_2)},$$

where each of the terms on the right-hand side is guaranteed to exist since it involves only jointly measurable quantities. This joint probability distribution recovers all the measurable marginals $p(A_i = a_i, B_j = b_j)$. Notice that the no-signaling principle is crucial to the above derivation as it ensures that $p(B_1 = b_1, C_2 = c_2)$ derived as the marginal probability from $p(A_1 = a_1, B_1 = b_1, C_2 = c_2)$ is the same as that derived from $p(A_2 = a_2, B_1 = b_1, C_2 = c_2)$. This independence of the measurement outcomes on settings chosen in a distant location is precisely the condition imposed by the no-signaling principle. Therefore, each of the Bell inequalities represented by $B(A_1, A_2, B_1, C_2)$ and $B(A_1, A_2, B_2, C_1)$ cannot be violated in any theory obeying the no-signaling principle. Consequently, these two quantities each are guaranteed to obey the local realistic bound of R (=2 in this CHSH case) in any no-signaling theory, leading to

$$B(A_1, A_2, B_1, C_2) + B(A_1, A_2, B_2, C_1) \leq 2R.$$

This guarantees by the previous arguments that

$$B(A_1, A_2, B_1, B_2) + B(A_1, A_2, C_1, C_2) \leq 2R. \tag{3.3}$$

We have therefore succeeded in deriving the monogamy relation Ineq. 3.3 that holds for the Bell-CHSH violations in any no-signaling theory. The construction can be readily extended to more systems and more measurements as well. The above method for the derivation of Bell monogamies can be stated as follows. Given a commutation graph representing a set of Bell inequalities, we look for a decomposition of this graph into subgraphs that each represent a Bell expression with known local realistic bound, such that a joint probability distribution can be found for all the measurements in the subgraph.

Let us emphasize that the monogamy relations derived above only arise under certain specific conditions, namely (i) Alice tries to violate the very same Bell inequality with all Bobs; (ii) Alice uses the same settings to violate Bell inequalities with all Bobs; (iii) No communication between Alice and Bob and between different Bobs is allowed; (iv) Each Bob cannot use more measurement settings than the total number of Bobs. Condition (i) and (ii) are strict conditions that stipulate that Alice tries to violate the same Bell inequality with all the different Bobs (in the CHSH scenario, the position of the negative sign in the Bell expressions must be the same), and uses the outcomes from the same measurement settings to do so. Condition (iii) is the assumption that no signaling between the different parties has taken place and condition (iv) is specific to the outlined method in that the proof technique (of decomposing the sum of Bell expressions into subgraphs that are themselves Bell expressions having a joint probability distribution) only works when the number of settings involved for a particular Bob is less than the total number of Bobs.

As a brief aside, let us mention that for the CHSH inequalities, within quantum theory condition (ii) can be relaxed. This this can be seen numerically as follows. We first write the general form of the pure state of a three qubit system as

$$|\psi_3\rangle = \sum_{i_1,i_2,i_3=0}^{1} \alpha_{i_1,i_2,i_3} |i_1, i_2, i_3\rangle$$

The coefficients α_{i_1,i_2,i_3} are complex numbers with the normalization condition imposing that their moduli sum to one, $\sum_{i_1,i_2,i_3} |\alpha_{i_1,i_2,i_3}|^2 = 1$. We then write the general observables on the qubits held by Alice, Bob and Charlie in terms of the Pauli matrices as $A_1 = \sigma_x$, $A_2 = a_x\sigma_x + a_y\sigma_y$, $A'_1 = {a'^1}_x\sigma_x + {a'^1}_y\sigma_y$, $A'_2 = {a'^2}_x\sigma_x + {a'^2}_y\sigma_y$, $B_1 = \sigma_x$,

$B_2 = b_x\sigma_x + b_y\sigma_y$, $C_1 = \sigma_x$, $C_2 = c_x\sigma_x + c_y\sigma_y$, with $k_x^2 + k_y^2 = 1$, $k = a, b, c, a'^1, a'^2$. Note that here Alice is no longer restricted to perform the same measurements A_1, A_2 for both Bell experiments instead choosing A'_1, A'_2 for the experiment with Charlie. That these observables are general is due to the fact that any two observables in this system lie in a plane, and the freedom to choose the first observable held by each party to be σ_x arises from the freedom in the choice of α_{i_1,i_2,i_3}. We then calculate the Bell-CHSH expressions $B(A_1, A_2, B_1, B_2)$ and $B(A'_1, A'_2, C_1, C_2)$ and maximize numerically over the variables. This procedure gives the monogamy result that $B(A_1, A_2, B_1, B_2) + B(A'_1, A'_2, C_1, C_2) \leq 4$ allowing the relaxation of the condition that Alice is required to choose the same measurement settings for violation of the Bell inequality with both Bob and Charlie, albeit only within quantum theory.

We now turn to the derivation of monogamies based on the no-signaling principle for multipartite Bell inequalities (where each inequality involves more than two parties). As we have seen, the method for the derivation of no-signaling monogamies relies on the vertex decomposition of the commutation graph now denoting a set of J Bell inequalities of N particles each into a series of J subgraphs each corresponding to a single Bell inequality. The idea behind this being that in each of the subgraphs, every particle (apart from the specific one held by Alice) is assigned a single measurement setting at most. When such a decomposition can be found, a joint probability distribution exists for each of the J subgraphs following the construction as before and the no-signaling bound for each of them is equal to the local realistic bound. Consequently, a monogamy relation analogous to the Ineq. (3.3) can be derived in this situation as well.

For the vertex decomposition of the commutation graph to exist, we require that there be at least as many parties as settings in each of the $N-1$ branches of the graph corresponding to the rest of the parties other than Alice. A simple instance of the no-signaling monogamy in the multipartite case can then be formulated as follows. Consider the violation of J Bell inequalities each of which involves N-particles (in general qudits) with n measurement settings per particle and has local realistic bound R. Let us assume there are a total of at least $n^{N-1} + 1$ particles involved in the experiment and that the number of Bell inequalities considered is $J = n^{N-1}$. Let us divide the particles into N sets $\vec{A}^{(i)}$ $(i = 1, \ldots, N)$ and let p_i denote the number of qudits in set $\vec{A}^{(i)}$. We choose $p_1 = 1$ (indicating a single Alice) and $p_j \geq n$ for $j = 2, \ldots, N$ (such that the number of parties is greater than the number of settings in each set). In the situation when each particle is involved in n Bell inequalities, the total number of Bell inequalities considered would be $J = n^{N-1}$. Then, by the method outlined previously, it can be seen that the violation of the monogamy relation

$$\sum_{p_1,p_2,\ldots,p_N} B(\vec{A}^{(1)}_{p_1}\vec{A}^{(2)}_{p_2}\ldots\vec{A}^{N}_{p_N}) \leq n^{N-1}R$$

implies signaling. Note that when more than n^{N-1} inequalities are considered, a no-signaling monogamy relation can be obtained by averaging over elementary monogamy relations such as the one above. Having established monogamy relations within no-signaling theories, we now proceed to identify the principle behind the appearance of monogamies within quantum theory. As in the CHSH scenario, we expect that the monogamies within quantum theory are stronger than those within general no-signaling theories.

3.4 Bell monogamy relations within Quantum theory

In this section, we demonstrate that monogamy of Bell inequality violations by quantum states can be derived on the basis of a principle which we refer to as "correlation complementarity".

3.4.1 Correlation Complementarity

We begin with the principle of complementarity, which forbids simultaneous knowledge of certain observables within quantum theory. The quintessential examples of such complementarity is between observables such as position and momentum for which as is well known, an uncertainty relation can be formulated. Here, we will focus on complementary observables for many-qubit systems.

Let us first demonstrate that the only dichotomic complementary observables (the outcomes of dichotomic observables take one of two values) within quantum theory are those that anti-commute. Consider a set of dichotomic (± 1) complementary measurements. The complementarity is manifested in the fact that if the expectation value of one measurement is ± 1 then expectation values of all other complementary measurements are zero. We show that the corresponding quantum mechanical operators anti-commute. Consider a pair of dichotomic operators A and B and assume that the expectation value $\langle A \rangle = 1$, i.e., the state being measured, say $|a\rangle$, is one of the $+1$ eigenstates of A. Complementarity requires $\langle a| B |a\rangle = 0$, which implies $B|a\rangle = |a_\perp\rangle$, where $\perp$ denotes a state orthogonal to $|a\rangle$. Since B is a dichotomic operator, $B^2 = \mathbb{1}$. We also have $B|a_\perp\rangle = |a\rangle$ and therefore $|b\rangle = \frac{1}{\sqrt{2}}(|a\rangle + |a_\perp\rangle)$ is the $+1$ eigenstate of B. For this state complementarity demands, $\langle b| A |b\rangle = 0$, i.e. $A|b\rangle$ is orthogonal to $|b\rangle$ which is only satisfied if $|a_\perp\rangle$ is the -1 eigenstate of A. The same argument applies to all the $+1$ eigenstates, therefore the two eigenspaces have equal dimension. As a consequence, $A = \sum_a (|a\rangle\langle a| - |a_\perp\rangle\langle a_\perp|)$ and $B = \sum_a (|a_\perp\rangle\langle a| + |a\rangle\langle a_\perp|)$. It is now easy to verify that A and B anti-commute. We have thus shown that the dichotomic complementary observables A and B necessarily anti-commute. We now use this fact to formulate the following Lemma, which we call the correlation complementarity principle.

Lemma {Correlation Complementarity principle}:

Consider a set of traceless and trace orthogonal dichotomic Hermitian operators A_k that obey $\{A_k, A_j\} = 2\delta_{k,j}\mathbb{1}$. Then their expectation values for any quantum-mechanical state ρ obey $\sum_k (tr[A_k\rho])^2 \leq 1$.

Here $\delta_{k,j}$ denotes the Kronecker delta symbol, i.e. $\delta_{k,j} = 1$ when $k = j$ and 0 otherwise.

Proof:

Consider a set S_k of dichotomic Hermitian operators A_k that obey the conditions in the Lemma. We denote by α_k their expectation values in some quantum-mechanical state ρ. These are real numbers in the range $[-1, +1]$. Construct an operator $F = \sum_{k=1}^{|S_k|} \alpha_k A_k = \vec{\alpha}.\vec{A}$. Now, $F^2 = |\vec{\alpha}|^2\mathbb{1}$ due to the anti-commutativity condition $\{A_k, A_j\} = 2\delta_{k,j}\mathbb{1}$. Also, the expectation value of F in state ρ is given by $\langle F\rangle = |\vec{\alpha}|^2$. Therefore, since the variance of this Hermitian operator in state ρ given by $\langle F^2\rangle - \langle F\rangle^2$ must be positive if ρ is to be a physical state, we obtain that $|\vec{\alpha}|^2(1 - |\vec{\alpha}|^2) \geq 0$ or in other words,

$$|\vec{\alpha}|^2 = \sum_k (tr[A_k\rho])^2 \leq 1. \tag{3.4}$$

This completes the proof.

As a result of the Correlation complementarity principle, we see that if the expectation value of any dichotomous observable is ± 1 in a state, then the expectation values in the same state of all dichotomous observables that anti-commute with it are necessarily zero. Thus, anti-commuting operators encode the concept of complementarity in the quantum formalism. We note that the above Lemma was also obtained in Refs. [60, 61] with a different proof. Also observing that for dichotomic observables, the square of the expectation value is related to the Tsallis entropy as $S_2(A_k) = \frac{1}{2}(1 - \langle A_k\rangle^2)$, the inequality in the Lemma can be converted into an entropic uncertainty relation. Here we focus on using this uncertainty relation for studies of non-locality, such as deriving the Tsirelson bound (an application also noted in [62]) and in particular for the derivation of the Bell monogamy relations for qubits.

3.4.2 Derivation of Bell Monogamies from Complementarity

In this section, we outline a method for the derivation of BMR's within quantum theory using the correlation complementarity principle. We will focus our attention on the complete collection of two-setting correlation Bell inequalities for N qubits formulated in [63]. There, it was shown that all these Bell inequalities can be condensed into a single general Bell inequality given as

$$\sum_{s_1,\ldots,s_N=-1,1} \left| \sum_{k_1,\ldots,k_N=1,2} s_1^{k_1-1} \ldots s_N^{k_N-1} E(k_1, \ldots, k_N) \right| \leq 2^N. \tag{3.5}$$

Here, the indices k_j denote the two possible measurement settings for each of the N observers and $E(k_1, \ldots, k_N)$ denotes the multipartite correlation function, the average correlation in the measurement outcomes.

The non-violation of this general Bell inequality was shown to be a necessary and sufficient condition for the correlations in the two-setting (for each party) Bell experiment to admit a local hidden variable (LHV) description. This is in contrast to a single inequality like the CHSH inequality, the satisfaction of which does not guarantee the existence of an LHV description. For the case of two qubits, if the general Bell inequality is satisfied, then all CHSH inequalities are satisfied. A sufficient condition for the violation of this general Bell inequality was derived. We first explain this condition and then use the correlation complementarity principle to derive BMR's for qubits.

A general N-qubit density matrix can be decomposed into tensor products of Pauli operators

$$\rho = \frac{1}{2^N} \sum_{\mu_1,\ldots,\mu_N=0}^{3} T_{\mu_1\ldots\mu_N} \sigma_{\mu_1} \otimes \cdots \otimes \sigma_{\mu_N},$$

where $\sigma_{\mu_n} \in \{\mathbb{1}, \sigma_x, \sigma_y, \sigma_z\}$ is the μ_n-th local Pauli operator for the n-th party and $T_{\mu_1\ldots\mu_N} = tr[\rho(\sigma_{\mu_1} \otimes \cdots \otimes \sigma_{\mu_N})]$ are the components of the correlation tensor $\hat{T}$. In the following, we will use both notations $\mu_n = 0, 1, 2, 3$ and $\mu_n = 0, x, y, z$ for convenience where there is no possibility of confusion. The orthogonal basis of tensor products of Pauli operators has the property that its elements either commute or anti-commute. It was shown in [63] that the correlations between the measurements on N qubits satisfy the general Bell inequality (3.5) if and only if in any set of local coordinate system of the N observers and for any set of unit vectors $\vec{c}^j = (c_1^j, c_2^j)$ one has

$$\sum_{x_1,\ldots,x_N=1,2} c^1_{x_1} \ldots c^N_{x_N} \left|T_{x_1\ldots x_N}\right| \leq 1.$$

By then applying the Cauchy inequality, the following useful and simple sufficient condition for the local realistic description of the correlation functions for N qubits was derived. If in every set of local coordinate systems of N observers, one has

$$\sum_{x_1,\ldots,x_N=1}^{2} T^2_{x_1\ldots x_N} \leq 1,$$

then the correlations between the measurements on N qubits satisfy the general Bell Inequality (3.5).

In other words, the quantum value of the general Bell parameter (normalized so that the local realistic bound is one), denoted by $\mathcal{L}$, was shown to have an upper bound of

$$\mathcal{L}^2 \leq \sum_{k_1,\ldots,k_N=x,y} T^2_{k_1\ldots k_N}, \tag{3.6}$$

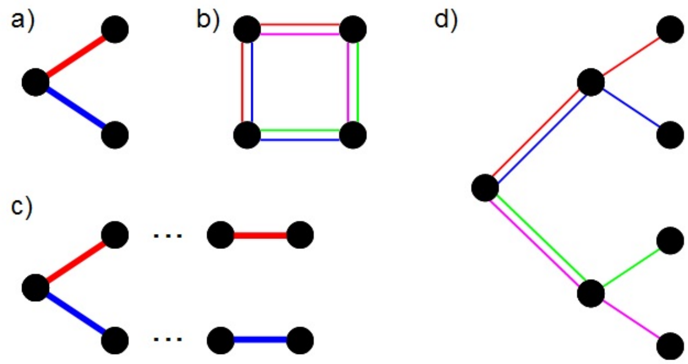

Figure 3.3: The nodes of these graphs represent observers trying to violate Bell inequalities which are denoted by colored edges. **(a)** The simplest case: two subsets of three parties try to violate CHSH inequality. **(b)** Four three-party subsets of four parties try to violate Mermin inequality. **(c)** Two subsets of odd number of parties try to violate a multi-partite Bell inequality when only one particle is common to two Bell experiments. **(d)** A binary tree configuration leading to a strong monogamy relation.

where summation is over orthogonal local directions x and y which span the plane of the local settings [63]. The above condition is sufficient for the existence of an LHV model for two-setting Bell experiments, if the upper bound above is smaller than the classical limit of 1, there exists an LHV model. Our method for finding quantum bounds for Bell violations is to use condition (3.6) for combinations of Bell parameters and then identify sets of anti-commuting operators in order to utilize inequality (3.4) and obtain a bound on these combinations.

We begin by showing an application of Inequality (3.4) from the correlation complementarity principle to a derivation of the Tsirelson bound (applications of this inequality to deriving Tsirelson bounds were also considered in [62]). For two qubits, the general Bell parameter is upper bounded by $\mathcal{L}^2 \leq T_{xx}^2 + T_{xy}^2 + T_{yx}^2 + T_{yy}^2$. One can identify here two vectors of averages of anti-commuting observables, e.g., $\vec{\alpha}_1 = (T_{xx}, T_{xy})$ and $\vec{\alpha}_2 = (T_{yx}, T_{yy})$. Due to (3.4) we obtain $\mathcal{L} \leq \sqrt{2}$ which is exactly the Tsirelson bound (when the local realistic bound is 2, one recovers the more commonly used value of $2\sqrt{2}$. One can apply this method to look for corresponding maximal quantum violations of other correlation inequalities, e.g. it is easy to verify that the "Tsirelson bound" of the multi-setting inequalities [64] is just the same as the one for the two-setting inequalities.

Our derivation shows that Tsirelson's bound is due to complementarity of correlations $T_{ix}^2 + T_{iy}^2 \leq 1$ with $i = x, y$. Any theory more non-local than quantum mechanics would have to violate this complementarity relation, related results were obtained in [65]. This relation can be generalized, e.g., for two qubits there is a set of five mutually anti-commuting operators leading to $T_{ix}^2 + T_{iy}^2 + T_{iz}^2 + T_{j0}^2 + T_{k0}^2 \leq 1$ with $i \neq j \neq k$.

To see how complementarity of correlations can be used to establish Bell monogamy, consider the simplest scenario of three particles, illustrated in Fig. (3.3a). We show that if correlations obtained in two-setting Bell experiment by AB cannot be modeled by LHV, then correlations obtained by AC admit LHV model. We use condition (3.6) which applied to the present bipartite scenario reads: $\mathcal{L}_{AB}^2 + \mathcal{L}_{AC}^2 \leq \sum_{k,l=x,y} T_{kl0}^2 + \sum_{k,m=x,y} T_{k0m}^2$. It is important to note that the settings of party A are the same in both sums and accordingly orthogonal local directions x and y are the same for A in both sums. We arrange the Pauli operators corresponding to correlation tensor components entering the sums into the following two sets of anti-commuting operators: $\{XX\mathbb{1}, XY\mathbb{1}, Y\mathbb{1}X, Y\mathbb{1}Y\}$ and $\{YX\mathbb{1}, YY\mathbb{1}, X\mathbb{1}X, X\mathbb{1}Y\}$, where $X = \sigma_x$ and $Y = \sigma_y$. Note that the anti-commutation of any pair of operators within a set is solely due to anti-commutativity of local Pauli operators. We then obtain the result that $\mathcal{L}_{AB}^2 + \mathcal{L}_{AC}^2 \leq 2$. Once a CHSH inequality is violated between AB, all CHSH inequalities between AC are satisfied, reproducing similar results that were obtained in [43, 45].

Before we move to a general case of arbitrary number of qubits, we present an explicit example of multipartite monogamy relation. Consider parties A, B, C, D trying to violate a correlation Bell inequality in a scenario depicted in Fig. (3.3b). We show the new monogamy relation: $\mathcal{L}_{ABC}^2 + \mathcal{L}_{ABD}^2 + \mathcal{L}_{ACD}^2 + \mathcal{L}_{BCD}^2 \leq 4$. Condition (3.6) applied to these tripartite Bell parameters implies that the left-hand side is bounded by the sum of 32 elements. The corresponding tensor products of Pauli operators can be grouped into four sets:

$$
\begin{aligned}
&\{XXY\mathbb{1}, XY\mathbb{1}X, X\mathbb{1}XY, \mathbb{1}YYY, \dots\},\\
&\{XYX\mathbb{1}, YY\mathbb{1}Y, Y\mathbb{1}XX, \mathbb{1}XXY, \dots\},\\
&\{YXX\mathbb{1}, XX\mathbb{1}Y, Y\mathbb{1}YY, \mathbb{1}XYX, \dots\},\\
&\{YYY\mathbb{1}, YX\mathbb{1}X, X\mathbb{1}YX, \mathbb{1}YXX, \dots\},
\end{aligned}
$$

where the dots denote four more operators being the previous four operators with X replaced by Y and vice versa. All operators in each set anti-commute, therefore the bound of 4 is proved.

To give a concrete example of monogamy of a well-known inequality we choose the inequality due to Mermin [66]: $E_{112} + E_{121} + E_{211} - E_{222} \leq 2$, where E_{klm} denote the correlation functions for measurement settings k, l and m. Since the classical bound of the Mermin inequality is 2, and not 1 as we have assumed in our derivation, the new "Mermin monogamy" is $\mathcal{M}_{ABC}^2 + \mathcal{M}_{ABD}^2 + \mathcal{M}_{ACD}^2 + \mathcal{M}_{BCD}^2 \leq 16$, where $\mathcal{M}$ is the quantum value of the corresponding Mermin parameter. The bound of the new monogamy relation can be achieved in many ways. If a triple of observers share the GHZ state, they can obtain maximal violation of 4 and the remaining triples observe vanishing Mermin quantities $\mathcal{M}$. This can be attributed to maximal entanglement of the GHZ state. It is also possible for two and three triples to violate Mermin inequality non-maximally, and at the same time to achieve the bound. For example, the state $\frac{1}{2}\left(|0001\rangle + |0010\rangle + i\sqrt{2}|1111\rangle\right)$ allows ABC and ABD to obtain $\mathcal{M} = 2\sqrt{2}$, and the state $\frac{1}{\sqrt{6}}\left(|0001\rangle + |0010\rangle + |0100\rangle + i\sqrt{3}|1111\rangle\right)$ allows ABC, ABD and ACD to obtain $\mathcal{M} = \frac{4}{\sqrt{3}}$. Note that it is impossible to violate all four inequalities simultaneously.

We now derive new monogamy relations for N qubits. Consider the scenario of Fig. (3.3c), in which N is odd, A is the fixed qubit and the remaining $N-1$ qubits are split into two groups $\vec{B} = (B_1, ..., B_M)$ and $\vec{C} = (C_1, ..., C_M)$ each containing $M = \frac{1}{2}(N-1)$ qubits. We shall derive the trade-off relation between violation of $(M+1)$-partite Bell inequality by parties $A\vec{B}$ and $A\vec{C}$. Using condition (3.6), the elements of the correlation tensor which enter the bound of $\mathcal{L}^2_{A\vec{B}} + \mathcal{L}^2_{A\vec{C}}$ are of the form $T_{kl_1...l_M0...0}$ and $T_{k0...0m_1...m_M}$. The corresponding Pauli operators can be arranged into 2^M sets of four mutually anti-commuting operators each: $\vec{A}_{1S} = \{XXSI, XYSI, YIXS, YIYS\}$, $\vec{A}_{2S} = \{YXSI, YYSI, XIXS, XIYS\}$, where S stands for all 2^{M-1} combinations of X's and Y's for $M-1$ parties, and $I = \mathbb{1}^{\otimes M}$ is identity operator on M neighboring qubits. Therefore, according to the theorem, we arrive at the following trade-off: $\mathcal{L}^2_{A\vec{B}} + \mathcal{L}^2_{A\vec{C}} \leq 2^M$.

The bound of this inequality is tight in the sense that there exist quantum states achieving the bound for all allowed values of $\mathcal{L}_{A\vec{B}}$ and $\mathcal{L}_{A\vec{C}}$. This is a generalization of a similar property for CHSH monogamy [45]. The state of interest can be chosen as

$$|\psi\rangle = \tfrac{1}{\sqrt{2}}\cos\alpha\left(|0\vec{0}\vec{0}\rangle + |1\vec{0}\vec{1}\rangle\right) + \tfrac{1}{\sqrt{2}}\sin\alpha\left(|1\vec{1}\vec{0}\rangle + |0\vec{1}\vec{1}\rangle\right), \tag{3.7}$$

where e.g. $|1\vec{0}\vec{1}\rangle$ denotes a state in which qubit A is in the $|1\rangle$ eigenstate of local Z basis, all qubits of $\vec{B}$ are in state $|0\rangle$ of their local Z bases, and all qubits of $\vec{C}$ are in state $|1\rangle$ of their respective Z bases. The non-vanishing correlation tensor components in xy plane, which involve only $(M+1)$-partite correlations are $T_{x\vec{w}\vec{0}} = \pm\sin 2\alpha$, $T_{x\vec{0}\vec{w}} = \pm 1$, and $T_{y\vec{0}\vec{v}} = -\cos 2\alpha$, where $\vec{w}$ contains even number of y indices, other indices being x, and $\vec{v}$ contains odd number of y indices, other indices again being x. There are $\sum_{k=1}^{\lfloor M/2 \rfloor}\binom{M}{2k} = 2^{M-1}$ correlation tensor elements of each type and consequently

$$\mathcal{L}^2_{A\vec{B}} = 2^{M-1}\sin^2 2\alpha, \quad \mathcal{L}^2_{A\vec{C}} = 2^{M-1}(1+\cos^2 2\alpha).$$

Therefore, the bound is achieved for all α and all allowed values of $\mathcal{L}_{A\vec{B}}$ and $\mathcal{L}_{A\vec{C}}$ can be attained either by the state (3.7) or the state with the role of qubits $\vec{B} \leftrightarrow \vec{C}$ interchanged.

The underlying reason why the above trade-off allows for violation by both $A\vec{B}$ and $A\vec{C}$ is the fact that sets of anti-commuting operators of the Bell parameters can contain at most four elements. Now we present a much stronger monogamy related to the graph in Fig. (3.3d). Consider M-partite Bell inequalities corresponding to different paths from the root of the graph to its leaves ($M = 3$ in Fig. (3.3d)). There are 2^{M-1} such inequalities and we shall prove that their quantum mechanical values obey

$$\mathcal{L}_1^2 + \cdots + \mathcal{L}_{2^{M-1}}^2 \leq 2^{M-1}, \tag{3.8}$$

where $\mathcal{L}_j$ is the quantum value for the j-th Bell parameter in the graph. To prove this, we construct 2^{M-1} sets of anti-commuting operators, each set containing 2^M elements, such that they exhaust all correlation tensor elements which enter the bound of the left-hand side of (3.8) after application of condition (3.6). The construction also uses the graph of the binary tree. We begin at the root (the left most qubit), to which we associate a set of two anti-commuting operators, X and Y, for the corresponding qubit. A general rule now is that if we move up in the graph from qubit A to qubit B we generate two new anti-commuting operators by placing X and Y at position B to the operator which had X at position A. Similarly, if we move down in the graph to qubit C we generate two new anti-commuting operators by placing X and Y at position C to the operator which contained Y at position A. For example, starting from the set of operators (X, Y) by moving up we obtain $(XX\mathbb{1}, XY\mathbb{1})$, and by moving down we have $(Y\mathbb{1}X, Y\mathbb{1}Y)$. The next sets of operators are $(XX\mathbb{1}X\mathbb{1}\mathbb{1}\mathbb{1}, XX\mathbb{1}Y\mathbb{1}\mathbb{1}\mathbb{1})$, $(XY\mathbb{1}\mathbb{1}X\mathbb{1}\mathbb{1}, XY\mathbb{1}\mathbb{1}Y\mathbb{1}\mathbb{1})$, $(Y\mathbb{1}X\mathbb{1}\mathbb{1}X\mathbb{1}, Y\mathbb{1}X\mathbb{1}\mathbb{1}Y\mathbb{1})$ and $(Y\mathbb{1}Y\mathbb{1}\mathbb{1}\mathbb{1}X, Y\mathbb{1}Y\mathbb{1}\mathbb{1}\mathbb{1}Y)$ if we move from the root: up up, up down, down up and down down, respectively. By following this procedure in the whole graph we obtain a set of 2^M mutually anti-commuting operators. According to this algorithm the anti-commuting operators can be grouped in pairs having the same Pauli operators except for the qubits of the last step (the leaves of the graph). There are 2^{M-1} such pairs corresponding to distinct combinations of tensor products of X and Y operators on $M-1$ positions. Importantly, in different operators these positions are different and to generate the whole set of operators entering the bound we have to perform suitable permutations of positions. Such permutations always exist and they do not affect anti-commutativity. Finally we end up with the promised 2^{M-1} sets of 2^M anti-commuting operators each, which according to Ineq. (3.4) from the correlation complementarity give the bound of (3.8).

The inequality (3.8) is stronger than the previous trade-off relation in the sense that it does not allow simultaneous violation of all the inequalities of its left-hand side. All other patterns of violations are possible as we now show. Choose any number, m, of Bell inequalities, i.e. paths in the Fig. (3.3d). Altogether they involve n parties which share the following quantum state

$$|\psi_n\rangle = \frac{1}{\sqrt{2}}|\underbrace{0\ldots0}_{n}\rangle + \frac{1}{\sqrt{2m}}\sum_{j=1}^{m}|0\ldots0\underbrace{1\ldots1}_{\mathcal{P}_j}0\ldots0\rangle,$$

where $\mathcal{P}_j$ denotes parties involved in the j-th Bell inequality. Note that all states under the sum are orthogonal as they involve different parties. The only non-vanishing components of the correlation tensor of this state have even number of y indices for the parties involved in the Bell inequalities. Squares of all these components are equal to $\frac{1}{m}$ which gives $\mathcal{L}_j^2 = \frac{2^{M-1}}{m}$ for each Bell inequality $j = 1, \ldots, m$. Therefore, all m Bell inequalities are violated as soon as $m < 2^{M-1}$. Moreover, the sum of these m Bell parameters saturates the bound of (3.8) and therefore independently of the state shared by other parties the remaining Bell parameters of (3.8) all vanish.

3.5 General bipartite Bell monogamies

In this section, we use the method illustrated in the examples in Fig. (3.3) to find general monogamies for bipartite inequalities in any configuration. Consider N observers each having access to a single qubit. They are asked to violate a set of bipartite Bell inequalities, this problem is represented by a graph G having observers as vertices and inequalities as edges. An example of such a graph is given in Fig. (3.4). It turns out that the simplest scenario of Bell monogamy plays a crucial role in understanding the features of the monogamy for an arbitrary such graph.

The simplest Bell monogamy involves three parties in a configuration where Alice A tries to simultaneously violate a Bell inequality with Bob B and Charlie C. The statement of Bell monogamy is that the simultaneous violation is impossible and the quantitative relation of Ineq. (3.2) is restated as

$$\mathcal{L}_{AB}^2 + \mathcal{L}_{AC}^2 \leq 2. \tag{3.9}$$

For a general graph we can now use the following method to derive a tight Bell monogamy relation. A line graph L of the initial graph G is constructed by placing vertices of L on every edge of G, and connecting the vertices of L whenever the corresponding edges of G share a vertex (Fig.(3.4)). In the figure, the graph G is denoted by black edges and circles for the vertices, while its line graph L is represented by red edges and square vertices. The properties of the line graph L determine the Bell monogamy relations. Note that Bell inequalities are now represented by vertices of L and edges of L tell us when two Bell inequalities share a common observer. In other words for every edge of L we have an elementary monogamy relation (3.9). Summing up the monogamy relations corresponding to all edges of L we obtain

$$\sum_v d_v \mathcal{L}_v^2 \leq 2\varepsilon, \tag{3.10}$$

where the sum is over the vertices of L, d_v denotes the degree of vertex v, i.e. the number of edges incident to the vertex, $\mathcal{L}_v$ is the Bell parameter related to vertex v and ε is the number of edges in L. The factor of 2 comes from the elementary monogamy relation (3.9).

The monogamy relation (3.10) is tight in the sense that the bound cannot be any smaller. This follows from the well-known Handshaking Lemma [67] in graph theory

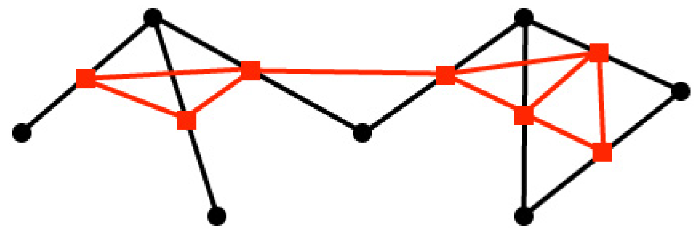

Figure 3.4: General monogamy involving bipartite Bell inequalities. In the black graph G, vertices denote observers and edges connect observers in a bipartite Bell experiment. Red graph L is the line graph of G with vertices denoting Bell inequalities and edges connecting experiments sharing a common observer.

stating that for any finite undirected graph $\sum_v d_v = 2\varepsilon$. This corresponds to $\mathcal{L}_v = 1$ for all the vertices of L, which is exactly the local hidden variable bound achievable for all the vertices. This therefore provides a complete characterization of tight monogamies for general bipartite Bell inequality violations.

Apart from being tight, i.e. there exist a quantum state and suitable measurements which saturate the bound, the elementary Bell monogamy relation (3.9) has another interesting feature we might call *spherical tightness*. We identify a monogamy relation as being spherically tight if all algebraically allowed values of Bell operators that saturate its bound can be realized by suitable quantum states and measurements. Since the relations we are discussing are quadratic functions of Bell parameters, the resulting shape is a hypersphere and hence the terminology.

Spherical tightness of (3.9) was shown for the first time in [45], but here we shall give a different example that is useful for studies of many other monogamies. Consider the following state of three qubits

$$|\psi\rangle = \frac{1}{\sqrt{2}}(\alpha_1 |001\rangle + \alpha_2 |010\rangle + |111\rangle),$$

with reals α_j summing up as $\alpha_1^2 + \alpha_2^2 = 1$. The bound for $\mathcal{L}_{AB}^2$, computed for the marginal state ρ_{AB}, is now given by $2\alpha_1^2$ and it is known that it can be achieved with suitable measurements [42]. In the next step, note the marginal density operator ρ_{AC} is given by that of ρ_{AB} in which one replaces $\alpha_1 \leftrightarrow \alpha_2$, and therefore keeping the same settings for A and allowing C to choose the same settings as those of B, we arrive at $\mathcal{L}_{AC}^2 = 2\alpha_2^2$. In this way the spherical tightness is proved for the elementary monogamy relation (3.9). However, this is the only monogamy in the bipartite case that is spherically tight as can be seen by the following argument. In general, every bipartite Bell parameter satisfies the Tsirelson bound $\mathcal{L}_v^2 \leq 2$. Therefore, the general monogamy relation (3.10) is not spherically tight if at least one $d_v < \varepsilon$ because the corresponding inequality cannot reach the 2ε bound. This is indeed the case as the only graph with all $d_v = \varepsilon$ has two vertices and one edge, i.e. it is the line graph of the generating monogamy relation.

3.6 Conclusions and Open Questions

In this chapter, we have investigated the phenomenon of monogamy of Bell inequality violations, deriving the constraint on the violations imposed by the no-signaling principle as well as the stronger constraint imposed by the complementarity principle in quantum mechanics. In particular, we have demonstrated a method for the derivation of monogamy relations within quantum theory based on the identification of complementary observables within all the Bell parameters considered in a monogamy experiment. Using the method, we derived tight monogamy relations for bipartite as well as multipartite Bell inequality violations in the typical scenario where each observer holds a qubit and performs one of two measurements on it.

While a complete characterization of the monogamies in the case of bipartite inequalities has been achieved, such a characterization for the case of multipartite inequalities remains to be performed. Another important open problem is the extension of the methods to the scenario where the observables are not dichotomic, i.e, where the measurements in each Bell experiment have more than two outcomes. Possible extensions to more than two measurements per observer would also be useful. It would also be interesting to see if the trade-offs can be derived without using the quantum formalism at all, a possible candidate for this task being the principle of information causality [68]. Finally, some applications of the intriguing phenomenon of monogamy have been identified; in the next chapter we apply these monogamy relations to show how a local realistic description emerges for the correlations in everyday macroscopic systems.

Chapter 4

Macroscopic Local Realism

We have been studying one of the cornerstone principles distinguishing quantum theory from classical theories, the notion of local realism. The famous paper by Einstein, Podolsky and Rosen (EPR) [1] in 1935 was titled "Can quantum-mechanical description of physical reality be considered complete?". In that paper, EPR postulated a criterion for a quantity to be an element of physical reality in the following manner: "If, without in any way disturbing a system, we can predict with certainty (i.e., with probability equal to unity) the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity". The notion of realism thus posits that measurable properties of physical systems exist before measurements are performed. In their argument that the quantum mechanical wave function does not provide a complete description of the physical system, EPR also used the notion of locality. This states that measurements on one system cannot influence the outcomes of measurements in a spatially separated second system (or in any system that is not interacting with the first). Using entangled quantum states of two particles (a precursor to the arguments by John Bell as outlined in the previous chapter), EPR arrived at a contradiction by showing that both the position and momentum of a particle must be elements of reality, so that it should be possible to assign definite values to them in contrast to the Heisenberg uncertainty principle. They thus concluded that quantum mechanics is an incomplete theory in need of further refinement to make it in accord with local realism. In fact, the lack of realism in quantum theory troubled EPR as can be seen from the following quote attributed to Einstein "Do you really believe the Moon is not there when nobody looks?". In other words, the question is whether the position of the Moon should be considered an element of reality. In this chapter, we study whether the correlations in macroscopic objects such as the Moon display the lack of local realism present in the underlying quantum theory.

As we have seen in the previous chapter, John Bell in 1964 used simple reasoning to formulate an algebraic inequality (Bell inequality) to demonstrate that local realism is in contradiction with the predictions of quantum theory [4]. His work brought the question of the completeness of quantum theory and the necessity of local realism in physical theories to the experimental domain. Numerous experiments have since been performed which unequivocally support quantum theory while showing that a local realistic description of the microscopic world is untenable. Various loopholes, which potentially still allow a local realistic description of the measured data, were closed individually [69, 52, 53, 54, 70, 71]. Although there is still no conclusive experiment closing all the loopholes at the same time, there is almost unanimous agreement that on the microscopic scale the world is *not* local realistic. In other words, while quantum mechanics could be superseded by more advanced theories, it is not necessary to complete it to bring it in accord with local realism, since Nature at the microscopic level does not conform to local realism.

The macroscopic world we experience is on the contrary described by classical physics, a local realistic theory. A fundamental question one could ask is how a local realistic macroscopic world emerges from the microscopic scale, on which level it cannot be described by local realism. A number of resolutions to this question have been suggested. The more radical ones, the so-called collapse models [72, 73, 74, 75, 76, 77], predict that quantum mechanics will fail for sufficiently complex systems. Another approach is to look for classicality as a limit of quantum phenomena. The well-known decoherence program stipulates that superpositions of macroscopic states such as the pointer state of a measuring apparatus are suppressed by an inevitable interaction between the quantum system and its environment, see for instance [78, 79, 80]. A conceptually different approach focuses on the limits of observability of quantum effects in macroscopic objects [81, 82, 83, 84]. Here we follow, albeit in a slightly different manner to that in the literature, the last of the stated approaches to the question.

The steady progress in experimental techniques allows one to perform measurements that were considered infeasible decades ago. Experiments have reached a level of sophistication where several spins can be manipulated coherently for sufficiently long times to perform small quantum computations [85]. In spite of this tremendous progress, one still faces a formidable challenge to manipulate individual components in systems consisting of a macroscopic number (say of the order of the Avogrado number 10^{23}) of particles. Although one cannot exclude such a possibility in the future, at the present moment it is simply an experimental impossibility and there might even be fundamental reasons why such manipulations may never be possible [86]. This lack of addressability of each individual particle in a macroscopic system is at the heart of the development of classical and quantum statistical mechanics as tools to describe such systems (a typical often studied example is the system of particles in an ideal gas).

In this chapter, we will consider the nature of the correlations that can reasonably be measured on macroscopic systems, and show that if the number of measured particles is large enough, a local realistic description emerges, regardless of the quantum state of the system. Note that local realism of the correlations does not rule out entanglement in macroscopic systems, which is another manifestation of quantum weirdness that is not equivalent with local realism [55] (indeed, highly entangled states between macroscopic systems have been prepared in the lab, for instance [87]). The intuition behind this result is that macroscopic measurements do not reveal the properties of individual particles, and quantum correlations are monogamous [43, 44, 58, 88, 26, 27] while classical correlations are not. The monogamy of quantum correlations implies that while individual subsystems within the macroscopic object can violate a Bell inequality, the averaging over many such inequalities brought about by macroscopically feasible measurements gives rise to a local realistic description for the total system. The local realistic macroscopic limit we will derive is more general than classical physics itself and it is an interesting open problem to identify classical physics within the set of local realistic theories. The material covered in this chapter includes a detailed exposition of the results presented by the author and collaborators in [89], as well as a detailed algorithm to derive macroscopic local realism from the correlation complementarity principle.

4.1 Macroscopically feasible measurements

Consider a macroscopic sample composed of many microscopic spins, this being a good approximation to many macroscopic systems such as magnetic materials and metals [90]. While we restrict ourselves to spin systems here, our considerations can also be extended to other systems. We are interested in experimentally feasible measurements performed on macroscopic regions of the system whose results can be known with arbitrary precision. By macroscopically feasible measurements, we mean those that cannot address individual microscopic particles.

The simplest observables of this kind are different directions of magnetization in macroscopic parts of the system, where magnetization is the average projection of all spins in a given direction. For example, for spin-$\frac{1}{2}$ particles, the magnetization observables are described by one-body operators that can be written as $\sum_k \vec{n} \cdot \vec{\sigma}_k$, with $\vec{\sigma}_k = (\sigma_x, \sigma_y, \sigma_z)_k$ being the standard Pauli operators acting on the kth particle and $\vec{n}$ being a 3-component vector of unit length. One could also consider M-body observables that read $\sum_\kappa O_\kappa$, where κ contains all different subsets of M particles and O_κ is an arbitrary M-qubit Hermitian operator. These are increasingly hard to implement experimentally with increasing M (or to extract from the measurement results of single-body operators, as would be the case with the variance, which is a two-body operator). For this reason, we focus on magnetization measurements as the most feasible scenario and later we extend our considerations to the case of M-body measurements to show that they do not change our central results, up to some high M threshold.

The outcome of a magnetization measurement does not reveal information about the spin projections of individual particles; there are many configurations of individual spin projections that give rise to the same total magnetization. The situation is therefore analogous to statistical mechanics, where one macrostate is realized by the averaging over an enormous number of microstates. Moreover, in a realistic experiment such as that performed in [91], where a macroscopic region of the sample is measured, one obtains directly the average value of magnetization with vanishingly small fluctuations without many repetitions of the experiment. The detailed probability distribution that determines the average value is, for all practical purposes, inaccessible.

When measured on the sample, a macroscopic observable gives almost always the same outcome being its average. We stress that the results we will derive on local realism for any macroscopic quantum state apply to these average values of macrosopic correlations such as those measured in [91] and not to the detailed probability distribution. Indeed, one may consider a more general scenario such as in [92], where a macroscopic beam of particle pairs is sent through the measurement apparatus of two spatially separated parties and intensities are measured at a number of detectors corresponding to different outcomes. In that scenario, while the detailed probability distribution of the various outcomes is still unavailable, one may consider some resolution of the detectors giving information on the intensity fluctuations at each detector. In [92], it was shown that for fluctuations of the order of square root of the number of particle pairs N, the central limit theorem can be used to derive a local hidden variable model for the correlations in states of the form $\sigma^{\otimes N}$, where σ denotes the state of a single particle pair. In this regard, while our results apply to all multipartite quantum states, it must be noted that the derivation of LHV models for the detailed probability distribution of measurement outcomes is left as an open question. With this caveat, we now proceed to the derivation of LHV models for macroscopic correlations.

4.2 Macroscopic correlations admit LHV description

We investigate a lattice of macroscopically many qubits, $N \approx 10^{23}$, prepared in some state ρ, and aim to prove the existence of a local hidden variable model for the correlations between magnetization measurements on macroscopic regions of these qubits. Before moving to the general case however, we illustrate the application of the monogamy results of the previous chapter to the simplest such scenario. Consider dividing the lattice into two disjoint regions A and B, as depicted in Fig. (4.1), containing N_A and N_B qubits respectively, where N_A, N_B are of the order of N. In each of the regions, we perform a measurement of local magnetizations $\mathcal{M}_{\vec{a}}$ ($\mathcal{M}_{\vec{b}}$) along some directions $\vec{a}$ ($\vec{b}$):

$$\mathcal{M}_{\vec{a}} \equiv \sum_{i \in A} \vec{a} \cdot \vec{\sigma}_i \quad \text{and} \quad \mathcal{M}_{\vec{b}} \equiv \sum_{j \in B} \vec{b} \cdot \vec{\sigma}_j. \tag{4.1}$$

Quantum correlations between the magnetization measurements for the system in the state ρ, $\mathbb{E}_{\vec{a}\vec{b}} = \langle \mathcal{M}_{\vec{a}} \otimes \mathcal{M}_{\vec{b}} \rangle_\rho$, are given by the sum of microscopic correlations between all pairs of qubits from different regions:

$$\mathbb{E}_{\vec{a}\vec{b}} = \sum_{i\in A}\sum_{j\in B} tr\left[(\vec{a}\cdot\vec{\sigma}_i \otimes \vec{b}\cdot\vec{\sigma}_j)\rho\right]. \tag{4.2}$$

One crucial observation is that the very same measurements are performed on all the microscopic pairs (the assumption of macroscopic feasibility), so that the macroscopic magnetization correlations are effectively described by the averaged state of two qubits:

$$\mathbb{E}_{\vec{a}\vec{b}} = N_A N_B tr\left[(\vec{a}\cdot\vec{\sigma} \otimes \vec{b}\cdot\vec{\sigma})\rho_{eff}^{AB}\right], \tag{4.3}$$

where the effective two-qubit state is described by the positive semi-definite operator

$$\rho_{eff}^{AB} = \frac{1}{N_A N_B}\sum_{i\in A}\sum_{j\in B}\rho_{ij}, \tag{4.4}$$

and ρ_{ij} is the reduced density matrix for i^{th} qubit at A and j^{th} qubit at B. These different expectation values can then be combined together using coefficients $\alpha(\vec{a},\vec{b})$ for the S_A, S_B different measurement settings on Alice's and Bob's partitions respectively, to give what we might refer to as a macroscopic Bell parameter:

$$\langle\mathcal{B}\rangle = \sum_{\vec{a},\vec{b}}\alpha(\vec{a},\vec{b})\mathbb{E}_{\vec{a}\vec{b}}.$$

In general, any set of correlations $\mathcal{E}_{\vec{a}\vec{b}}$ admits a local hidden variable model (LHV) if there are parameters λ, distributed with some probability density $\mu(\lambda)$, and local response functions $J_A(\vec{a},\lambda)$ and $J_B(\vec{b},\lambda)$ such that

$$\mathcal{E}_{\vec{a}\vec{b}} = \int d\lambda\mu(\lambda)J_A(\vec{a},\lambda)J_B(\vec{b},\lambda). \tag{4.5}$$

Applying this to our scenario, the set of quantum correlations $\mathbb{E}_{\vec{a}\vec{b}}$ admits an LHV model if it is possible to construct such a model for correlations obtained from the effective state ρ_{eff}^{AB}. Therefore, ρ_{eff}^{AB} will be the focus of our study.

Another important observation is that whatever results we succeed in deriving regarding a set of states ρ which do not violate some class of macroscopic Bell inequalities, will apply equally to the class of states $(\prod_{i=1}^{N_A}U_i^A\prod_{j=1}^{N_B}U_j^B)\rho(\prod_{i=1}^{N_A}U_i^A\prod_{j=1}^{N_B}U_j^B)^\dagger$ for measurement settings $U_i^A(\vec{a}\cdot\vec{\sigma})U_i^{A\dagger}$ and $U_i^B(\vec{b}\cdot\vec{\sigma})U_i^{B\dagger}$ under the same conditions. For instance, if we prove that no state ρ violates a set of Bell inequalities, this instantly generalizes to Bell inequalities which allow for some variation of magnetic fields over the sample since the variation in magnetic fields can be translated into a transformation of the state ρ.

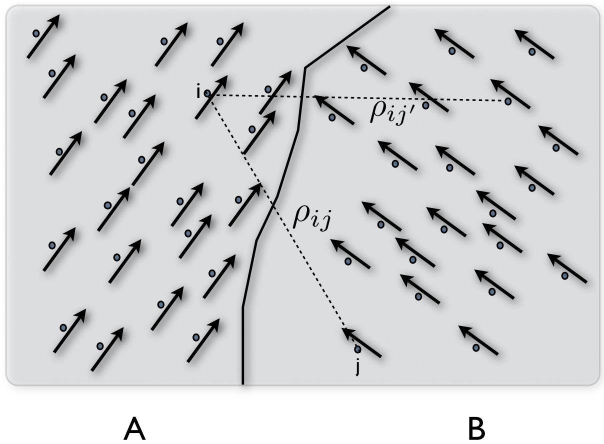

Figure 4.1: Measurements of local magnetization in macroscopic regions A and B. The monogamous nature of quantum correlations limits the strength of correlations in states ρ_{ij} and $\rho_{ij'}$ that share a common qubit i.

4.3 Explicit models and quantum complementarity

In this section, we will show that ρ_{eff}^{AB} admits LHV description for two magnetization measurements performed on two macroscopic regions of the sample and generalize the result in the next section for a number of regions up to $\log_2 N$. Our proof will proceed by utilizing the quantum character of the magnetization measurements, but makes no assumption on the behavior of correlations which do not enter into the magnetization outcomes. In this way, the conclusions of this section stay unchanged even if some day quantum theory should be found to disagree on some mesoscopic scale with experimental data of measurements other than magnetization.

We now make use of the monogamy results from the previous chapter. As seen there, a set of four correlations measured on a two-qubit state with one of two local observables admits an explicit LHV model [63] if elements of the correlation tensor $T_{kl} = tr\left[\sigma_k \otimes \sigma_l \rho\right]$ satisfy [63]:

$$\mathcal{L} \equiv \sum_{k,l=x,y} T_{kl}^2 \leq 1, \tag{4.6}$$

where orthogonal local directions x and y are defined to be along the sum and difference of the two local setting vectors. Note that this condition does not require orthogonal measurement settings in the Bell experiment.

We apply this condition to the effective state ρ_{eff}^{AB}. The elements of its correlation tensor read

$$T_{kl} = \frac{1}{N_A N_B} \sum_{i \in A} \sum_{j \in B} T_{kl}^{(ij)}, \tag{4.7}$$

where $T_{kl}^{(ij)}$ is the component of the correlation tensor of the state ρ_{ij}. Substituting into (4.6) gives

$$\mathcal{L} = \frac{1}{N_A^2 N_B^2} \sum_{i,i' \in A} \sum_{j,j' \in B} \vec{T}^{(ij)} \cdot \vec{T}^{(i'j')}, \tag{4.8}$$

with $\vec{T}^{(ij)} = (T_{xx}^{(ij)}, T_{xy}^{(ij)}, T_{yx}^{(ij)}, T_{yy}^{(ij)})$. In the next step, we write $\mathcal{L}$ as a combination of vectors $\vec{P}^{(ij)} = (T_{xx}^{(ij)}, T_{xy}^{(ij)}, T_{yx}^{(i(j+1))}, T_{yy}^{(i(j+1))})$ and $\vec{Q}^{(ij)} = (T_{xx}^{(i(j+1))}, T_{xy}^{(i(j+1))}, T_{yx}^{(ij)}, T_{yy}^{(ij)})$, the components of which are expectation values of mutually anti-commuting operators:

$$\mathcal{L} = \frac{1}{2N_A^2 N_B^2} \sum_{i,i' \in A} \sum_{j,j' \in B} \left(\vec{P}^{(ij)} \cdot \vec{P}^{(i'j')} + \vec{Q}^{(ij)} \cdot \vec{Q}^{(i'j')} \right). \tag{4.9}$$

The components of vectors $\vec{P}^{(ij)}$ and $\vec{Q}^{(ij)}$ involve correlations between two pairs of micro-systems, pair (ij) and $(i(j+1))$ where the sum is modulo N_B. The monogamous nature of correlations between these pairs, which stem from quantum complementarity, limits the lengths of $\vec{P}^{(ij)}$ and $\vec{Q}^{(ij)}$ below one (see chapter on Monogamy of Bell inequalities). We consequently derive $\mathcal{L} \leq 1$. This shows that the correlations between local magnetizations in the system of N qubits are of classical nature as long as N_A or N_B is greater than one. In effect, the quantum correlations get diluted in the effective state ρ_{eff}^{AB} due to monogamy between the different pairwise terms, which themselves arise because the observables see the whole quantum state ρ as an equally weighted average over all possible pairs of qubits between regions A and B.

We now generalize this method to the scenario where the system of N qubits is partitioned into K regions such that there are N_k, of the order of $\frac{N}{K}$, particles in each region, with $k = 1, \dots K$. We will then prove that when $K \leq \log_2(N)$ there is always an LHV description for all quantum states ρ. We stress that the bound on K may not be tight and even more macroscopic observers may still not be able to violate a Bell inequality.

The method can also be extended to the scenario where one measures M-body observables (magnetization being a 1-body observable), and consequently considers Bell inequalities of $2M$-qubit correlation functions. It can be shown using the above methods that in particular CHSH-like inequalities are not violated by macroscopic systems up to some high threshold M.

4.4 Multipartite Scenario

We generalize the simple derivation in the previous section to the scenario where the system of N qubits is partitioned into k regions, namely $A, B \dots K$ such that there are

N_k particles in each region. We temporarily assume that all N_k are equal to some n so that $N = n \times k$. The case where the number of particles in each region is different will be dealt with later. Once again, we consider the situation where the local magnetization is measured in each region. The question is then: Does a state ρ of the system exist such that the correlations between the local magnetizations are non-classical?

We now proceed in a manner analogous to the bipartite scenario. The correlations between local magnetizations read

$$\left\langle \mathcal{M}_{\vec{n}_1} \otimes \cdots \otimes \mathcal{M}_{\vec{n}_k} \right\rangle = n^k tr\left[(\vec{n}_1 \cdot \vec{\sigma} \otimes \cdots \otimes \vec{n}_k \cdot \vec{\sigma}) \rho_{eff}^{AB\ldots K} \right], \tag{4.10}$$

where the effective state is now a state between k qubits

$$\rho_{eff}^{AB\ldots K} = \frac{1}{n^k} \sum_{l_1 \in A} \cdots \sum_{l_k \in K} \rho_{l_1 \ldots l_k}$$

constructed from the k-qubit reduced density matrices, $\rho_{l_1 \ldots l_k}$, between qubits taken one from each region. The existence of an LHV model for k-qubit correlation measurements in this effective state then implies its existence for the whole quantum state ρ.

We once again use the results from [63] where it was shown that a set of 2^k correlation functions obtained on a k-qubit state by measuring one of two local observables admits an LHV model if

$$\sum_{i_1 \ldots i_k = \{x,y\}} T_{i_1 \ldots i_k}^2 \leq 1, \tag{4.11}$$

where $T_{i_1 \ldots i_k} = tr\left[(\sigma_{i_1} \otimes \cdots \otimes \sigma_{i_k}) \rho_{eff}^{AB\ldots K} \right]$ is the correlation function for the orthogonal local directions $\vec{x}$ and $\vec{y}$ defined as sum and difference of local measurement settings. In our problem, these correlation functions read

$$T_{i_1 \ldots i_k} = \frac{1}{n^k} \sum_{l_1 \in R_1} \cdots \sum_{l_k \in R_k} T_{i_1 \ldots i_k}^{l_1 \ldots l_k}, \tag{4.12}$$

where $T_{i_1 \ldots i_k}^{l_1 \ldots l_k}$ gives the correlations between a set of k particles labelled by $l_1 \ldots l_k$. Inserting this expression into the LHV criterion yields

$$\sum_{i_1 \ldots i_k = \{x,y\}} T_{i_1 \ldots i_k}^2 = \frac{1}{n^{2k}} \sum_{i_1 \ldots i_k = \{x,y\}} \left(\sum_{l_1 \ldots l_k} \sum_{l_1' \ldots l_k'} T_{i_1 \ldots i_k}^{l_1 \ldots l_k} T_{i_1 \ldots i_k}^{l_1' \ldots l_k'} \right). \tag{4.13}$$

We show under which conditions this expression is less than 1 in order to satisfy the LHV criterion.

This will be accomplished by showing that the expression above can be written as the sum of scalar products between every pair of n^k vectors each of which has length at most one. Note that the sums over $i_1 \ldots i_k$ and the sums over $l_1 \ldots l_k$ and $l_1' \ldots l_k'$ from

1 to N_k result in a total of $2^k \times n^{2k}$ terms in the above expression. Hence, each vector that we construct must have a minimum of 2^k components so that the final expression has magnitude less than 1. We know from the correlation complementarity that if the components of each vector are averages of mutually anti-commuting observables, the length of the vector is bounded by 1. The task then is to find n^k groups of 2^k correlation functions $T^{l_1 \dots l_k}_{i_1 \dots i_k}$ such that the corresponding observables $\sigma_{i_1} \otimes \cdots \otimes \sigma_{i_k}$ mutually anti-commute. This is achieved by a generalization of what was done in the bipartite scenario. Note that the total dimension of the Hilbert space for the entire system is $2^{nk} = 2^N$. It is known that in a system of dimension 2^N, there are at most $2N+1$ mutually anti-commuting observables. Hence, only when k is of order $\log_2 N$ (2^k is of order N) or less, we may hope to find the vectors of size 2^k containing mutually anti-commuting observables. We now present an algorithm to accomplish this task. We will first construct one vector of 2^k components and build the other $n^k - 1$ vectors by applying certain transformations to this vector.

For simplicity, we shall first construct the vector as a set of 2^k mutually anti-commuting observables and then replace the observables by the corresponding correlation functions. Note that each component of the vector is a tensor product of k single qubit observables of the type $\sigma_i^{l_j}$ acting on one of the qubits l_j on each region. For each qubit l_j in region J, these can take values $\sigma_x^{l_j}$ and $\sigma_y^{l_j}$ which directly anti-commute, or $\mathbb{1}^{l_j}$. Since we need 2^k mutually anti-commuting observables, one solution is to construct a binary tree algorithm which would require $N_k = 2^{k-1}$ qubits in region k. This is illustrated by the left figure in Fig. (4.2). The construction proceeds as follows. We first list all 2^k observables containing only the observables σ_x and σ_y at each position: $\sigma_x^{l_1} \otimes \cdots \otimes \sigma_x^{l_k}$ to $\sigma_y^{l_1} \otimes \cdots \otimes \sigma_y^{l_k}$. Construct each of the n^k vectors to contain all such strings, the difference between the vectors being only in the values of $l_1 \dots l_k$ chosen so as to obtain mutual anti-commutativity. In the tree algorithm depicted in the left figure Fig. (4.2), we see the construction of 16 mutually anti-commuting operators for $k = 4$ regions. In a given region R_j (with $j \in \{1, 2, 3, 4\}$), we let $l_j = 1, \dots, 2^{j-1}$. Each branch of the tree then represents one operator sequence and the 16 branches of the tree denote the 16 mutually anti-commuting operators. For clarity, we explicitly detail the construction below.

Region R_1 contains qubit 1, R_2 has two qubits (labeled 2 and 3), R_3 has four qubits (labeled $4, 5, 6, 7$) and region R_4 has eight qubits (numbered $8, 9, 10, 11, 12, 13, 14, 15$). The 16 mutually anti-commuting operators in the left diagram in Fig. (4.2) are:

$$
\begin{array}{llll}
\sigma_x^1 \otimes \sigma_x^2 \otimes \sigma_x^4 \otimes \sigma_x^8, & \sigma_x^1 \otimes \sigma_x^2 \otimes \sigma_x^4 \otimes \sigma_y^8, & \sigma_x^1 \otimes \sigma_x^2 \otimes \sigma_y^4 \otimes \sigma_x^9, & \sigma_x^1 \otimes \sigma_x^2 \otimes \sigma_y^4 \otimes \sigma_y^9, \\
\sigma_x^1 \otimes \sigma_y^2 \otimes \sigma_x^5 \otimes \sigma_x^{10}, & \sigma_x^1 \otimes \sigma_y^2 \otimes \sigma_x^5 \otimes \sigma_y^{10}, & \sigma_x^1 \otimes \sigma_y^2 \otimes \sigma_y^5 \otimes \sigma_x^{11}, & \sigma_x^1 \otimes \sigma_y^2 \otimes \sigma_y^4 \otimes \sigma_y^{11}, \\
\sigma_y^1 \otimes \sigma_x^3 \otimes \sigma_x^6 \otimes \sigma_x^{12}, & \sigma_y^1 \otimes \sigma_x^3 \otimes \sigma_x^6 \otimes \sigma_y^{12}, & \sigma_y^1 \otimes \sigma_x^3 \otimes \sigma_y^6 \otimes \sigma_x^{13}, & \sigma_y^1 \otimes \sigma_x^3 \otimes \sigma_y^6 \otimes \sigma_y^{13}, \\
\sigma_y^1 \otimes \sigma_y^3 \otimes \sigma_x^7 \otimes \sigma_x^{14}, & \sigma_y^1 \otimes \sigma_y^3 \otimes \sigma_x^7 \otimes \sigma_y^{14}, & \sigma_y^1 \otimes \sigma_y^3 \otimes \sigma_y^7 \otimes \sigma_x^{15}, & \sigma_y^1 \otimes \sigma_y^3 \otimes \sigma_y^7 \otimes \sigma_y^{15}
\end{array}
$$

Note that in each operator sequence, the qubits that do not appear in the sequence are

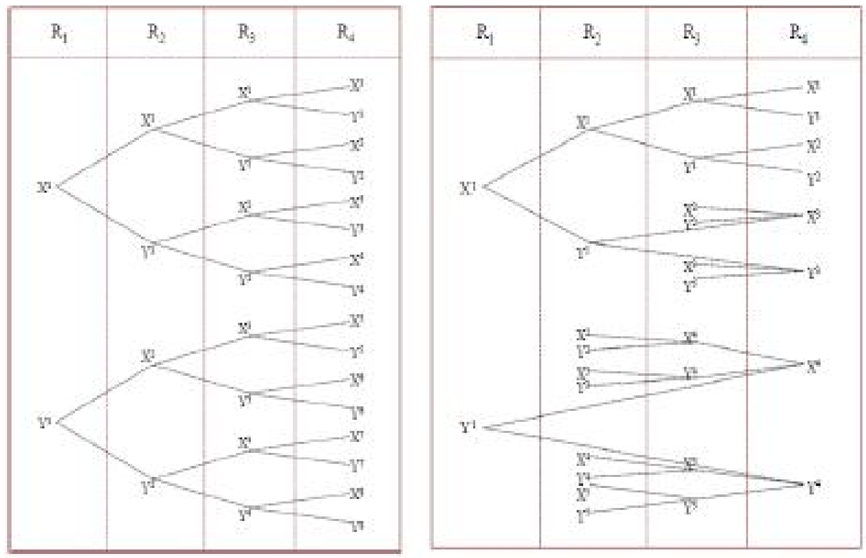

Figure 4.2: Left: Binary tree construction of 16 mutually anti-commuting operators for $k = 4$ regions. Here, σ_x (σ_y) has been labelled as X (Y). Each branch of the tree represents one operator sequence. For instance the top-most branch represents $\sigma_x^1 \otimes \sigma_x^1 \otimes \sigma_x^1 \otimes \sigma_x^1$. The number of particles in region J is then $N_j = 2^{j-1}$. Right: A factor k improvement on the number of particles per region can be obtained by folding the tree at particular operator sequences as explained in the text.

implicitly taken to have operator $\mathbb{1}$.

The remaining vectors are constructed by simple modifications to this initial vector. Two operations are performed: (i) change of l_j to l_{j+m} where addition is modulo m (this operation for each region j runs over all particles in the region); and (ii) change of σ_x to σ_y and vice versa. It is straightforward to show that these two operations applied to all operator sequences in a vector preserve the anti-commutation of operators. Moreover, all the n^k vectors can be obtained from one vector by applying these two operations. Hence, a possible grouping of terms is achieved which ensures that the LHV criterion is satisfied. The pitfall is that the algorithm is inefficient and needs one of the regions, namely the last one, to have $n = 2^{k-1}$ qubits. Since we assume that all regions contain roughly equal number of qubits, we have $N = 2^{k-1} \times k$.

A factor k improvement can be obtained by modifying the binary algorithm as we show below. First let us define a function $g(n)$ as the smallest power of 2 that is greater than or equal to n. We then define m to be $g(\frac{2^{k-1}}{k-1})$. We then carry out the binary tree algorithm for the first m operators with the leaf at the k^{th} region. In the second step, we shift the leaf of the tree one region to the left and construct the next m operators again by the binary tree method. Then in the third step, we shift the leaf one region to the left and construct $2m$ operators. In general, in the j^{th} step, we shift the leaf one region to the left and construct $2^{j-2} \times m$ operators by the binary tree method. We carry out this algorithm until 2^k operators are constructed at which point the binary string is exhausted and no more mutually anti-commuting operators exist. The algorithm thus describes a binary tree that curls back and equitably distributes the 2^k operators among the k regions giving at most $n = \sum_{l=1}^{k} g(\frac{2^{l-1}}{k-1})$ particles per grid. An illustration of this construction for $k = 4$ is given in the right diagram of Fig. (4.2). As before, other vectors are obtained from the first one constructed by applying the two operations previously described. A more careful reconstruction of the binary tree is possible to give $N_k \geq \left\lceil (\frac{2^{k-2}}{k-1}) \right\rceil$. This method therefore, assures us that given a sample with N qubits, a division into $k \leq \log_2(N)$ regions leads to a LHV model for magnetization measurements in two-setting Bell inequalities and more partitions are needed in order to violate such inequalities. We note that the binary tree method may not be optimal in constructing sets of mutually anti-commuting operators. One final point is that when the number of qubits in each region is different, $n = \left\lceil (\frac{2^{k-2}}{k-1}) \right\rceil$ represents the minimum number of qubits in any region that ensures the LHV model. It can be shown that the two operations described yield all vectors of mutually anti-commuting operators in this scenario as well.

4.5 LHV model of macroscopic correlations: General Proof

Having derived LHV models for correlations in macroscopic systems of qubits from the complementarity principle, we now turn our attention to the general scenario of arbitrary dimensional systems and general measurements. We divide a system of many spins into several regions $X = A, B, \ldots, K$ and study correlations between (generalized) magnetization observables in each region (see Fig. (4.3)). The spins can be of arbitrary local Hilbert space dimension, we only require that within a region X they are all of the same dimension d_X (qudits), and that there are N_X of them, enumerated by $x = 1, \ldots, N_X$. Within each region, we consider S_X sets of measurement operators (in general POVMs) $E_{i,j}^{X,x}$. Here the superscript X denotes the region X in which the measurement operator acts and x denotes the particle on which it is acting. The subscript i denotes the POVM element and j denotes the possible outcomes (of arbitrary number) of the measurement. Each set, indexed by i satisfies a completeness relation over the possible outcomes j such that $\sum_j E_{i,j}^{X,x} = \mathbb{1}_{d_X}$. These can be used to specify the operator of generalized magnetization in region X as

$$\mathcal{M}_i^X = \sum_{x=1}^{N_X} \sum_j f(j|i) E_{i,j}^{X,x}, \tag{4.14}$$

the usual magnetization being the case $f(j|i) = j$. We now assume, as a reflection of the macroscopic nature of the measurements, that POVM elements are the same for all particles within a region, and denote such elements as $E_{i,j}^X$ where the particle index is

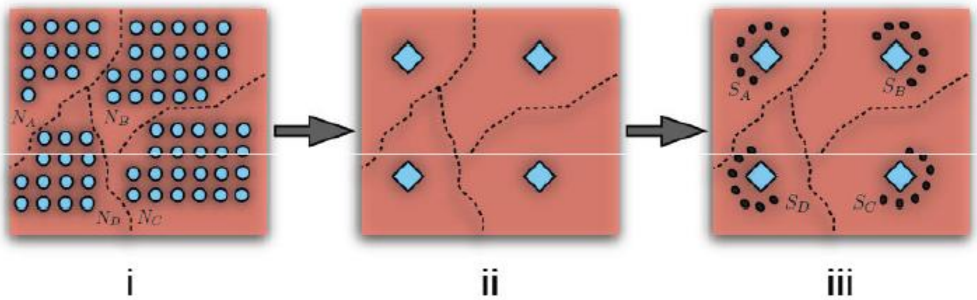

Figure 4.3: The three stages of the LHV strategy outlined in the text. (i) A system with four regions ($X = A, B, C, D$) of N_X particles (circles), measured with S_X different settings. The effective state ρ_{eff} for these measurements is shown in (ii) where squares depict effective particles. (iii) denotes the symmetric extension of ρ_{eff} to a state σ_N of S_X particles in each region; all the S_X measurements in each region X commute, implying the existence of a joint probability distribution and an LHV model for the state in (i).

skipped. Due to this assumption, the correlations between macroscopic measurements in a state ρ, $\mathbb{E}_{\vec{i}} = \text{Tr}(\rho \mathcal{M}^A_{i_A} \otimes \cdots \otimes \mathcal{M}^K_{i_K})$, are described by an effective positive semi-definite operator of only K spins

$$\rho_{\text{eff}}^{AB\ldots K} = \frac{1}{N_A \ldots N_K} \sum_{a\in A \ldots k \in K} \rho_{ab\ldots k}, \tag{4.15}$$

where $\rho_{ab\ldots k}$ is the reduced density matrix of the original state ρ on just spins a to k, one from each region. Following the steps as in the previous sections, the formula for the correlations now reads

$$\mathbb{E}_{\vec{i}} = \left(\prod_{X=A}^{K} N_X \right) \sum_{\vec{j}} \left(\prod_{X=A}^{K} f(j_X | i_X) \right) P(\vec{j}|\vec{i}), \tag{4.16}$$

where $\vec{j} = (j_A, \ldots, j_K)$ is a vector of measurement outcomes and $P(\vec{j}|\vec{i}) = tr(\rho_{\text{eff}} E^A_{i_A, j_A} \otimes \cdots \otimes E^K_{i_K, j_K})$ gives the probability to obtain these outcomes if the effective state is measured with settings $\vec{i} = (i_A, \ldots, i_K)$.

Now we prove more general results using the slightly stronger assumption that quantum predictions are valid even for experiments that cannot be performed in practice. In practice, each microscopic constituent of a macroscopic system cannot be addressed, but we assume that the predictions of quantum mechanics hold true even if they could be addressed. Our approach closely follows the proof technique in [88] which proved the monogamy of Bell inequalities. Given the similar nature of proofs in [58], one expects that the results can be extended to discuss why general no-signaling theories would also appear classical, so that the results would not be limited to quantum mechanics.

We can write a rather generic Bell inequality (which includes those previously defined as a subset) in terms of

$$\langle \mathcal{B} \rangle = \sum_{\vec{i},\vec{j}} \alpha(\vec{i},\vec{j}) tr \left(\rho_{eff}^{AB\ldots K} (E^A_{i_A,j_A} \otimes E^B_{i_B,j_B} \otimes \ldots E^K_{i_K,j_K}) \right)$$

where $\vec{i}$ is a vector of the measurement settings $i_A \ldots i_K$ and $\rho_{eff}^{AB\ldots K}$ is the effective state on K spins. Now we will show that the following quantum probability distribution

$$p(\vec{i},\vec{j}) = tr \left(\rho_{eff}^{AB\ldots K} (E^A_{i_A,j_A} \otimes E^B_{i_B,j_B} \otimes \ldots E^K_{i_K,j_K}) \right),$$

admits an LHV model. This can be done provided the number of measurement settings, S_X, is equal to the number of spins in the partition, N_X for all $X \in \{A, B \ldots K\}$. To start, we define vectors $\vec{m}_X$ of S_X elements, which read like a script for a deterministic protocol of what measurement results to give for each measurement setting: if the measurement setting is i_X, element $m_X^{i_X}$ is what should be given as outcome j_X. With this in place, we are in a position of give the LHV strategy (see Fig. (4.3)) – a source of shared randomness between all the parties selects a set of vectors $\vec{m}_A, \vec{m}_B \ldots \vec{m}_K$ with probability $tr \left(\rho' (E^A_{\vec{m}_A} \otimes E^B_{\vec{m}_B} \otimes \ldots E^K_{\vec{m}_K}) \right)$ where ρ' is any quantum state that has the property that every k-qubit reduced density matrix drawn from one Alice, one Bob etc. is equal to $\rho_{eff}^{AB\ldots K}$ and where $E^A_{\vec{m}_A} = E^A_{1,m_A^1} \otimes E^A_{2,m_A^2} \otimes \ldots E^A_{S_A,m_A^{S_A}}$, (this is well defined if $S_A = N_A$). Having jointly selected these vectors, then the parties wait until they're told what their measurement setting i_X is, at which point they give the outcome $m_X^{i_X}$. If we use this strategy, the resultant probability distribution is

$$p(\vec{i},\vec{j}) = \sum_{\vec{m}_A \ldots \vec{m}_K} tr(\rho' E^A_{\vec{m}_A} \otimes E^B_{\vec{m}_B} \otimes \ldots E^K_{\vec{m}_K}) \delta_{m_A^{i_A}, j_A} \ldots \delta_{m_K^{i_K}, j_K},$$

which can be readily seen to be equal to the desired distribution by using the completeness relations of the POVM operators. So, this will lead us to conclude that if at least one example of a state ρ' exists, for a given $\rho_{eff}^{AB\ldots K}$, then the original state ρ cannot violate a macroscopic Bell inequality of $S_A = N_A$, $S_B = N_B \ldots$ settings. We can now construct ρ' from ρ as follows. Let Π_X be a permutation over all spins of a given partition X. Then construct ρ' as

$$\rho' = \frac{1}{|\Pi_A| \ldots |\Pi_K|} \sum_{\Pi_A \ldots \Pi_K} (\Pi_A \otimes \Pi_B \ldots \otimes \Pi_K) \rho (\Pi_A \otimes \Pi_B \ldots \otimes \Pi_K)^\dagger.$$

The result readily extends in two ways. Firstly, we observe that in the N_A measurement settings (for instance), any two can be set equal to each other, and the result still holds. Thus, in fact, the result holds provided all $S_X \leq N_X$. Secondly, we can examine many-body observables. For M-body observables, we can redefine the effective Bell inequality of ρ_{eff} to be over M physical spins in each partition (although this requires that those M-body observables can be applied to all possible subsets of M spins, whereas one might prefer to impose a locality constraint). This has the effect of simply rescaling the limiting number of Bell measurements to N_X/M, assuming this is an integer. So, a system of say 10^{23} particles divided into 10^7 partitions, and involving 10^7-body observables would still require at least 10^9 measurement settings to possibly measure some violation of a Bell inequality, which we can justifiably consider infeasible. In general, for a total of N particles with M-body observables measured in each of k regions, the number of measurement settings in the Bell inequality required to observe a violation is at least $\frac{N}{kM}$.

This no-go theorem gives a very strong bound on the degree of control we would need over large systems for there to possibly be a violation of a Bell inequality. Indeed, the bound is quite tight since it says that for two parties with $N_A = 1$ and $N_B = 1, 2$ with $S_A = S_B = 1, 2$ there cannot be a Bell violation, whereas one can show that there is a violation for $N_A = 1$ and $N_B = 1, 2$ with $S_A = S_B = 2, 3$ (the $N_B = 1$ case is just CHSH, the $N_B = 2$ case uses a 3-setting Bell inequality known as I_{3322} found in [93]). Another interesting feature, however, is that there are some classes of states which we can show will never violate these macroscopic Bell inequalities, no matter how many measurement settings are allowed, as we will see in the following section.

4.6 Rotationally invariant systems

Stronger results can be proved in the bipartite scenario for restricted classes of N-qubit states ρ, such as those which are rotationally invariant, i.e.,

$$\rho = U^{\otimes N} \rho (U^{\otimes N})^{\dagger}, \tag{4.17}$$

for all single qubit unitaries U. This is a wide class of physically important states such as thermal states of the Heisenberg model. Firstly, we notice that any reduced density matrix ρ_{ij} obtained from ρ satisfying (4.17) is rotationally invariant, i.e., $\rho_{ij} = U \otimes U \rho_{ij} U^{\dagger} \otimes U^{\dagger} = V_{ij} |\psi_-\rangle\langle\psi_-|_{ij} + (1 - V_{ij}) \frac{\mathbb{1}_i \otimes \mathbb{1}_j}{4}$ [55]. Thus, the effective state ρ_{eff}^{AB} inherits the same property:

$$\rho_{eff}^{AB} = V |\psi_-\rangle\langle\psi_-|_{AB} + (1 - V) \frac{\mathbb{1}_A \otimes \mathbb{1}_B}{4}, \tag{4.18}$$

where $-\frac{1}{3} \leq V \leq 1$. It was proven in [94] that for $-\frac{1}{3} \leq V \leq 0.66$ this state admits an LHV description for all sets of projective quantum measurements, the upper bound on this range can be extended to 2/3 by invoking the results of [95]. It is also known [96] that if $p \leq \frac{5}{12}$, there is no Bell inequality violation at all, even allowing for POVMs. From our prior description of ρ_{eff}^{AB}, we can see that $V = \frac{1}{N_A N_B} \sum_{ij} V_{ij}$ and, from the singlet monogamy relation (see chapter on Optimal Cloning), one can prove that $V \leq \frac{R_{ab}+2}{3R_{ab}}$

where $R_{ab} = \max(N_A, N_B)$. Thus, provided our sample contains more than two qubits, we cannot violate a macroscopic Bell inequality (of any number of settings) composed of projective measurements; if N_A $(N_B) \geq 8$, there are no Bell inequalities whatsoever that can be violated.

4.7 Conclusions and Open Questions

We have studied some of the conditions under which one can sustain a local realistic description of correlations between macroscopic measurements. The assumption of macroscopic feasibility imposes that these measurements cannot access individual constituents of a macroscopic sample and therefore, the correlations between these measurements are diluted by averaging. It is interesting to note that perhaps we perceive the world as local realistic because the measurements we use for the purpose (such as the intensity of light from an object) are constrained by this macroscopic feasibility. Our results are distinct from related ones in the literature as they apply to sharp measurements, arbitrary closed systems and show that local realistic macroscopic correlations emerge within quantum theory or in some cases even if certain quantum predictions are not valid. While our results apply to the average values of correlations in macroscopic systems, one may also consider the detailed probability distribution of measurement outcomes such as in [92]. An important open problem then is to formulate conditions on the measurements and information about the probability distribution required to observe violation of a Bell inequality in this scenario.

The observables we have considered possess certain symmetry properties such as permutation invariance among the different particles in the sample. An important problem is to formulate precisely the restrictions placed on observables by virtue of the macroscopic size of the system under consideration. Another interesting open question is to verify if the LHV description of the macroscopic sample would emerge for any underlying no-signaling distribution from the monogamies within all no-signaling theories [58]. The ultimate goal of these studies is to establish conditions under which not only local realism of the macroscopic world emerges out of the microscopic quantum world, but even classical Newtonian physics. We now turn our attention to a generalization of the local realistic paradigm that we have been studying so far, the phenomenon of (non-)contextuality.

Chapter 5

Contextuality: Tests and Monogamy

We have seen so far that while the microscopic world does not conform to the idea of local realism, the macroscopic world does appear to be local realistic. A macroscopic object such as a ball has as one of its physical properties its position, which we can measure using light scattered from it. It is then the classical view that the position of the ball is a well-defined property irrespective of whether we choose to measure it. Going beyond realism is a closely related feature of classical theories called non-contextuality. This is the idea that the outcomes of measurements on a system should be independent of any other measurements that may be performed alongside them. In our example, non-contextuality would imply that the outcome of the position measurement at a particular instant does not depend on whether the measurement was carried out alongside another measurement such as that of the velocity of the ball or its angular momentum. Indeed, it would be truly bizarre if the ball was seen to be at some position x when its position and velocity were measured but at a different position y if at the same time the experimenter had chosen to measure position and angular momentum instead. We shall see in this chapter that quantum theory is indeed bizarre in this sense.

Quantum mechanics is not a theory that incorporates realism. According to quantum mechanics, when a particle is not observed it does not possess physical properties that exist independent of observation. In fact, such physical properties arise due to the measurements performed upon the system. This means that a spin-1/2 particle does not possess definite values for properties such as spin in the x-direction (σ_x), spin in the y-direction (σ_y), etc. Given the quantum state of this particle, quantum mechanics provides the rules for the calculation of probabilities for possible measurement outcomes of σ_x, σ_y, etc. The probabilistic outcomes in quantum theory are not even analogous to those in classical probabilistic theories such as the outcomes of a coin toss. As we have seen, the Bell theorem rules out a (local) realistic (even if probabilistic) formulation of quantum theory.

In this sense, the lack of realism in quantum theory goes beyond the lack of determinism in the outcomes of quantum measurements.

In a contextual theory, the outcomes of measurements depend upon what contexts (defined by other jointly performable measurements) they are performed in. Let us illustrate this concept with another more mathematical example. Imagine a physical system on which an observable A exists that can be measured together with an observable B or with C but that B and C cannot be measured simultaneously. In quantum mechanics, this situation would be captured by the equations $[A, B] = [A, C] = 0$ and $[B, C] \neq 0$, where the square brackets indicate the commutator of the enclosed observables. Measurements of B and C are said to provide two different contexts for the measurement of A. In any non-contextual theory, the outcome of the measurement of A does not depend on whether it was measured together with B or with C. Fig. (5.1) illustrates this concept in more detail. In this figure, each ellipsoid denotes a set of mutually commuting observables. Observables in different sets do not commute. There exists a particular observable Λ that belongs to all three sets. The observable Λ can be measured in three different contexts, for instance it can be measured either with A_k or with B_1 or with C_3 so that the three observables A_k, B_1, C_3 provide three different contexts for the measurement of Λ. Note that the verification of quantumness via non-contextual inequalities (the term "non-contextual inequality" to denote inequalities that are satisfied in any non-contextual theory was first used in [97]) requires both commutativity that ensures contexts and non-commutativity that makes it impossible to perform simultaneous measurements in different contexts. The essence of contextuality is thus the inability to assign an outcome to A prior to its measurement, independently of the context in which it was performed. In this sense, non-contextuality implies realism, but not vice versa. One could imagine contextual realistic theories which would assign values to properties depending on the choice of context for their measurement.

As shown by Kochen and Specker (KS) [9], for all quantum systems of dimension three and above, there exist sets of measurements that are contextual (whose outcomes depend on which other measurements they are performed with). More precisely, KS were able to find a set of 117 projection operators such that it is not possible to attribute to them either value 0 or 1 in an unambiguous manner without mutual conflict. The Kochen-Specker theorem is complementary to Bell's theorem and rules out hidden variable theories that require the EPR elements of reality to be non-contextual (independent of measurement arrangement). In doing so, the KS theorem does away with the locality assumption and applies to a single system, and is in this sense a generalization of the Bell theorem. In fact, both these theorems have the same mathematical underpinning, namely the concept of a joint probability distribution as shown by Fine in [49]. In any theory that incorporates realism, there exists a joint probability distribution for the outcomes of measurements for all physical properties of the system. Let us explore this in more detail.

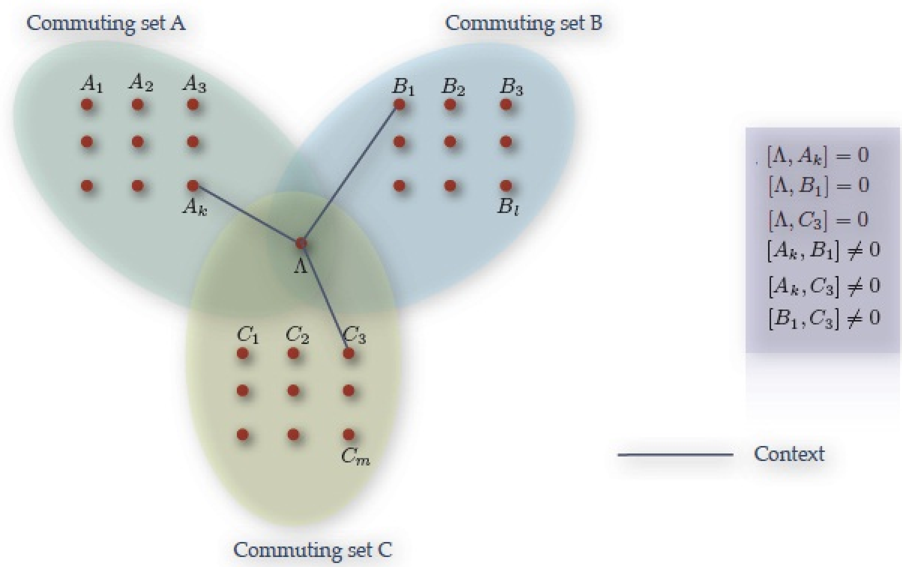

Figure 5.1: Illustration of the concept of contextuality. Each ellipse contains mutually commuting observables. A common observable Λ can be measured in different contexts such as with B_1 or with C_3 or with A_k.

Imagine a physical system on which a set of N measurements can be performed that are represented by some physical observables $A_1, A_2, \ldots, A_N$. Each observable A_i yields outcomes of measurements a_i with probability $p(A_i = a_i)$. Some of these observables are assumed to be jointly measurable, say $\{A_{k_1}, \ldots, A_{k_l}\}$ ($k_j \in \{1, \ldots, N\}$), yielding a set of outcomes $\{a_{k_1}, \ldots, a_{k_l}\}$ according to the respective joint probability distribution $p(A_{k_1} = a_{k_1}, \ldots, A_{k_l} = a_{k_l})$. Mathematically, realism requires that these joint probability distributions be the marginals of a *common* joint probability distribution of all observables, i.e., $p(A_1 = a_1, A_2 = a_2, \ldots, A_N = a_N)$ [49]. The existence of such a total joint probability distribution is non-trivial and depends on the probability distributions corresponding to all the possible subsets of jointly measurable observables. Local realism is then seen as a special kind of realism in which locality enables joint measurements. Contexts naturally arise under the locality assumption, since any two measurements in spatially separated locations can be jointly performed (within quantum theory such measurements always commute). From the point of view of joint probability distributions, the *non-contextuality* hypothesis is true if and only if there exists the joint probability distribution for the outcomes of all observations, i.e., $p(A_1 = a_1, A_2 = a_2, \ldots, A_N = a_N)$, such that one can recover all the experimentally measurable probabilities $p(A_{k_1} = a_{k_1}, \ldots, A_{k_l} = a_{k_l})$ as its marginals,

$$p(A_{k_1} = a_{k_1}, \ldots, A_{k_l} = a_{k_l}) = \sum_{\bar{a}_k} p(A_1 = a_1, \ldots, A_N = a_N).$$

Here the summation is over all the measurement outcomes excluding the set $\{a_{k_1}, \ldots, a_{k_l}\}$.

By showing that there exist observables within quantum theory that do not admit a joint probability distribution, Bell [4] and Kochen and Specker [9] were able to show that the property of realism is not present in quantum theory. As we have seen, the violation of a Bell inequality requires the state of the composite system held by the spatially separated parties, Alice and Bob, to be entangled. The Bell inequality by Clauser-Horne-Shimony-Holt (CHSH) [41] is the minimal experimental test of local realism requiring as it does two measurements each by Alice and Bob. In the case of contextuality, all quantum systems of a given dimension greater than two possess sets of contextual measurements, this is known as state-independent contextuality. For a given dimension of the quantum system, it is an ongoing enterprise to find the *minimal* set of measurements that reveal contextuality for any quantum state of that Hilbert space dimension. There are also state-dependent tests of contextuality, the test with the minimal number of measurements being the one proposed by Klyachko-Can-Binicoglu-Shumovsky (KCBS) [98] for quantum states of dimension three (qutrits). These tests are formulated in terms of inequalities that must be satisfied in any non-contextual theory and their violation implies the lack of non-contextual description for the measurements involved. In fact, for the spin-1 system (qutrit), the lack of the joint probability distribution has been experimentally confirmed in [99]. After the paper by Bell [4], many more Bell inequalities have been derived and extensively studied, for example [41, 100, 101]. Only a few extensions of the KCBS inequality have been proposed so far, for example [102, 103]. The fact that tests of local realism on physical systems require composite entangled systems and spatial separation while contextuality can be tested on a single system makes the study of contextuality an important and interesting line of research in understanding the quantumness of physical systems.

In this chapter, we begin by rigorously showing the minimality of 5 measurements for a state-dependent test of contextuality for a qutrit system. We then proceed to construct non-contextual inequalities based on the classical properties of the Shannon entropy. We then study how the concept of monogamy translates to non-contextual inequalities. Much of the material covered in this chapter follows the published works [104, 105], the methods though are described here in more lucid detail.

5.1 Non-Contextual Inequalities

In this section, we establish the minimal set of measurements that exhibit contextuality on the simplest contextual system, namely a qutrit (a three-level quantum system). After establishing that five cyclically commuting measurements are required to have a state-dependent test of contextuality in a qutrit [98], we show how non-contextual inequalities can be constructed using the information-theoretic notion of Shannon entropy of measurement outcomes. The minimality proof we present here is simpler and more direct than the one given in [106], the formulation of entropic inequalities for contextuality has also been explored in [103].

5.1.1 Pentagons are minimal

To show that quantum theory is a contextual theory, i.e. that it does not allow for a joint probability distribution, one needs more than two contexts as shown in [9]. A fundamental question for the existence of contextuality is to find the minimal number of measurements on some quantum system that one has to perform in order to observe contextuality. So far, the most economic proofs for a three-dimensional system (qutrit) consist of 5 measurements for a state-dependent test [98] and 13 measurements for a state-independent test [107]. Qutrits are of special interest since they are not only the smallest contextual systems, but they also physically correspond to a single system to which the concepts of nonlocality and entanglement cannot be unambiguously applied. Therefore, a single qutrit together with the most economical set of contextual measurements is a primitive of quantum contextuality similar to the system of an entangled pair of qubits and the CHSH (Clauser-Horn-Shimony-Holt) inequality [41] which is a primitive of quantum nonlocality.

We now find the minimal number of measurements required to reveal the contextuality of a single qutrit. One is tempted to start with two measurements A and B. However, this does not work because (i) either A and B commute in which case quantum mechanics itself provides a joint probability distribution (JPD) $p(A=a,B=b)=tr[(P_a^A\otimes P_b^B)\rho]$ where P_k^K is the projector onto the subspace corresponding to the value k of measurement K, or (ii) A and B do not commute and one can simply write $p(A=a,B=b)=p(A=a)p(B=b)$, which is a joint probability (albeit not within quantum mechanics) that reproduces the marginal probabilities $p(A)$ and $p(B)$ which are the only measurable probabilities in this scenario. Observe that a single particle on a straight line for which measurements of x (position) and p (momentum) do not commute is non-contextual as a consequence of case (ii). The next step is to consider three measurements: A, B and C. The various scenarios are as follows: (i) All three measurements mutually commute, which is equivalent to the case (i) above in the two measurement scenario in the sense that a JPD is provided within quantum theory, (ii) All of them do not commute, which allows us to define $p(A=a,B=b,C=c)=p(A=a)p(B=b)p(C=c)$ analogous to case (ii) for two measurements, (iii) Only one pair commutes (A and B say) in which case the JPD can be defined as $p(A=a,B=b,C=c)=p(A=a,B=b)p(C=c)$, where $p(A=a,B=b)$ is provided by quantum mechanics. We see in case (iii) again that while quantum mechanics does not itself provide the joint probability $p(A=a,B=b,C=c)$, nevertheless one may construct such a JPD recovering the experimentally measurable marginals. (iv) Only one

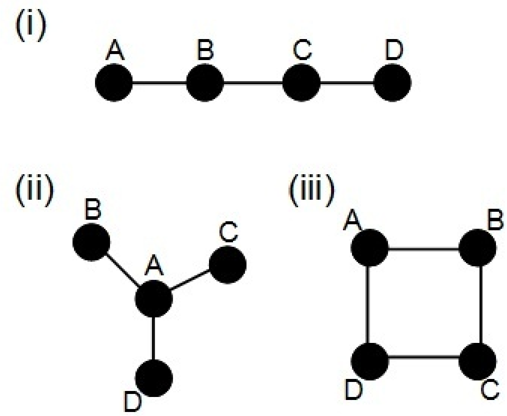

Figure 5.2: Graphical notation to represent the commutation relations between different observables. The commutation graphs (i)chain graph, (ii)star graph and (iii)cycle graph are shown.

pair (B and C say) does not commute in which case one may construct

$$p(A = a, B = b, C = c) = \frac{p(A = a, B = b)p(A = a, C = c)}{p(A = a)}.$$

This JPD again reproduces all the measurable marginals, therefore the system that has only two contexts is not sufficient to refute non-contextuality. The next case of four measurements was shown to be sufficient to prove this discrepancy for a system of dimension at least four, and is precisely the CHSH inequality [41].

Can we show the discrepancy for a three-level system and only four measurements? To show that the answer is no, it is convenient to introduce graphic notation as in Fig.(5.2) where the vertices of the graphs correspond to observables and edges between vertices represent commutativity, i.e., vertices representing observables A and B are connected if $[A, B] = 0$.

The only significant scenarios in the four measurement case that do not reduce to previous considerations are represented by the chain graph Fig.(5.2)(i), the star graph Fig.(5.2)(ii) and the cycle Fig.(5.2)(iii). For (i) we can construct

$$p(A = a, B = b, C = c, D = d) = \frac{p(A = a, B = b)p(B = b, C = c)p(C = c, D = d)}{p(B = b)p(C = c)},$$

and for (ii)

$$p(A = a, B = b, C = c, D = d) = \frac{p(A = a, B = b)p(A = a, C = c)p(A = a, D = d)}{p(A = a)^2}.$$

Note that the probabilities on the right-hand side of these equations exist due to the assumption of joint measurability. However for the graph in (iii), no four distinct measurements exist for a three-level system. This is because in order to have $[A, B] = 0$ and $[A, C] = 0$, but $[B, C] \neq 0$ one requires A to be a degenerate operator. In the case of a three-level system, this means that two eigenvalues of A are the same and therefore, without loss of generality A can be set to be a projector of rank one. Therefore all four measurements A, B, C and D are rank one projectors. The cycle graph (iii) implies that both A and C are orthogonal to B and D. Since we require that $B \neq D$ these two projectors span a plane orthogonal to both A and C which in three-dimensional Hilbert space implies $A = C$. The problem then reduces to the case (iii) for three measurements.

We have thus established that for three-level systems one requires at least five projective measurements to show the lack of joint probability distribution. Let us prove one property of the construction used above, namely that for any commutation graph which does not contain cycles (tree graph) there always exits a joint probability distribution consistent with quantum theory. This construction is given by the product of probability distributions corresponding to the edges of the graph (denoted by the set $E(G)$) divided by the product of probabilities of common vertices, where a vertex $i \in V(G)$ (the set of vertices of the graph) of degree $d(i)$ (the number of nearest neighbors) appears $d(i) - 1$ times in the product, i.e.,

$$p(A_1 = a_1, \ldots, A_N = a_N) = \frac{\prod_{(i,j)\in E(G)} p(A_i = a_i, A_j = a_j)}{\prod_{i\in V(G)} p(A_i = a_i)^{d(i)-1}}.$$

Since quantum theory provides joint probability distributions for any two commuting observables, this construction recovers any measurable marginal as can be seen by summing over the outcomes of all other observables, starting the summation from the leaves (free ends of the tree). For example, for the instance presented in Fig. (5.3)(i) the joint probability distribution is

$$p(A_1, \ldots, A_7) = \frac{p(A_1, A_2)p(A_1, A_3)p(A_2, A_4)p(A_2, A_5)p(A_3, A_6)p(A_3, A_7)}{p(A_1)p(A_2)^2 p(A_3)^2},$$

(where the outcomes are not explicitly mentioned for simplicity) and for instance to recover $p(A_2, A_5)$ the summation order is A_7, A_6, A_4, A_3, A_1.

Since all open graphs are trees for which joint probability distribution exists and for a three-level system one requires at least five projective measurements, the minimal graph for which one can show the discrepancy is a pentagon (5-cycle). For other graphs with cycles smaller than five, such as the example in Fig.(5.3)(ii), one can always find joint probability distributions, for example here

$$p(A_1, \ldots, A_5) = \frac{p(A_1, A_2, A_3)p(A_3, A_4)p(A_4, A_5)}{p(A_3)p(A_4)}.$$

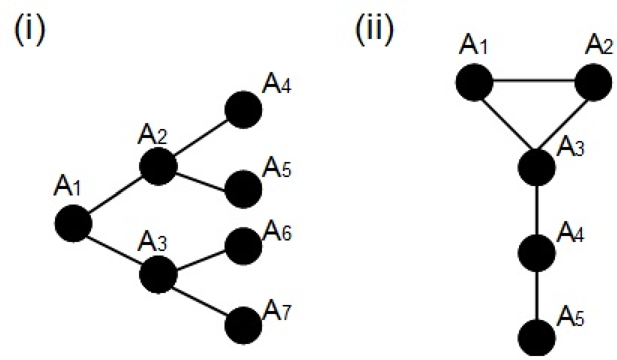

Figure 5.3: (i) Tree graph for seven observables and (ii) a graph with a single 3-cycle for five observables. Joint probability distributions can be derived for these graphs from the construction used in the text.

The similar case with a square (4-cycle) does not work due to reasons already discussed. This analytic result confirms the observation in [98] that projectors corresponding to the 5-cycle are necessary to reveal the contextuality of a single three-level system.

Before we proceed, let us extend the construction used above to formally prove that the class of chordal graphs admits a joint probability distribution. A chordal graph is a graph with no induced cycles of length greater than 3. By an induced cycle is meant a cycle that is an induced subgraph, i.e., between any two vertices of the subgraph there is an edge if and only if this edge was present in the original graph. This proposition implies that this large class of graphs cannot be used for tests of contextuality or for Kochen-Specker proofs.

Proposition 1:

A commutation graph G representing a set of n measurements for any n admits a joint probability distribution for these measurements if it is a chordal graph.

Proof:

The proof is by the construction illustrated previously. For notational convenience, in the probabilities we shall skip the outcomes that are left implicit. By assumption, the commutation graph G does not contain any induced cycles of length greater than 3. Let us denote the set of vertices of G by $V(G) = \{V_1, ..., V_n\}$. Let $K_3 = \{K_3^{(i)}\}$ denote the set of cycles of length 3 in G, $K_2 = \{K_2^{(i)}\}$ denote the set of edges (of length 2) in G that are not subgraphs of any graph $K_3^{(i)}$ and $K_1 = \{K_1^{(i)}\}$ denote the set of vertices (of length 1) in G that are not subgraphs of any graph $K_3^{(i)}$ or $K_2^{(i)}$. All the edges of the chordal graph G belong to one and only one of the sets K_1, K_2 or K_3 but they can occur more than once within a set. The vertices of G may appear in more than one set and also occur multiply within each set. Let $K = K_1 \bigcup K_2 \bigcup K_3$.

Then it is possible to construct the joint probability distribution for the set of n

measurements in G as

$$P(V_1, ..., V_n) = \frac{\Pi_{i=1}^{n(K_3)}\Pi_{j=1}^{n(K_2)}\Pi_{k=1}^{n(K_1)} P(K_3^{(i)})P(K_2^{(j)})P(K_1^{(k)})}{\Pi_{i<j=1}^{n(K)} P(K^{(i)} \bigcap K^{(j)})} \tag{5.1}$$

Here $n(K)$ denotes the number of elements in set K and $P(K^{(i)} \bigcap K^{(j)})$ denotes the probability of outcomes for the set of vertices that are at the intersection of the two elements $K^{(i)}$ and $K^{(j)}$. We can derive as the marginal probability of this joint probability distribution, any probability $P(K^{(i)})$ (of all experimentally measurable marginals) by summing over all elements other than $K^{(i)}$ in the following manner. We first carry out the summation of all elements $K^{(j)}$ whose intersection with $K^{(i)}$ is the null set. One can immediately see that in the resulting expression all the terms in the denominator $\Pi_{i<j=1}^{n(K)} P(K^{(i)} \bigcap K^{(j)})$ precisely cancel with all the terms in the numerator except $P(K^{(i)})$, thus recovering that marginal. This completes the proof.

It is now easy to see that Proposition 1 coupled with the fact that the measurements corresponding to a 4-cycle are not realizable in a quantum system of dimension three, imply that the five-cycle or the pentagon is the minimal measurement configuration to study the contextuality of the qutrit.

5.1.2 Entropic non-contextual inequalities

We now focus on the qutrit system and derive an entropic non-contextual inequality analogous to the entropic Bell inequality in [100]. It involves five projectors $\{A_1, A_2, \dots, A_5\}$ ($A_i = |A_i\rangle\langle A_i|$ has two outcomes $a_i = 0, 1$ and $i = 1, \dots, 5$) on which we impose cyclic orthogonality conditions, i.e. $A_i A_{i+1} = 0$, where we identify A_6 with A_1. Neighboring projectors are jointly measurable since they are orthogonal. As a result, for every projector A_i there exist two contexts: A_{i+1} and A_{i-1}. The commutation graph representing this scenario is the five-cycle graph shown in Fig.(5.4).

In [98], a non-contextual inequality was formulated using the average values of the projectors in the five-cycle graph as

$$\sum_{i=1}^{5} \langle A_i \rangle \leq 2. \tag{5.2}$$

Here the non-contextual bound of 2 is the independence number of the pentagon, where independence number refers to the maximal number of mutually disconnected vertices in the graph. That this number must be the non-contextual bound is seen as follows. Firstly, observe that we are dealing with quantities that can take two outcomes 0 and 1. If a particular quantity say A_2 takes the value 1 then immediately the quantities A_1 and A_3 are forced to take values 0 in any non-contextual theory. In a single experimental run measuring the five observables, the sum of the outcomes is the number of possible

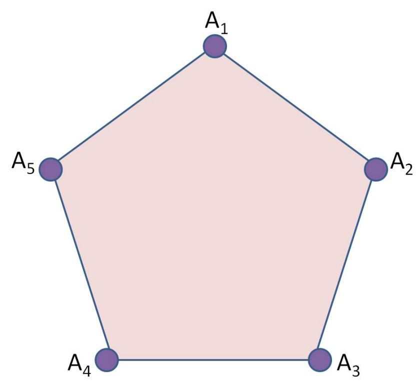

Figure 5.4: Pentagon graph showing the five projective measurements $A_1, \ldots, A_5$. Edges connect neighbouring vertices that commute, $A_i A_{i+1} = 0$.

outcomes 1 which is seen to be equal to the independence number of the graph. Now, if we average over many runs of the experiment, in the non-contextual theory

$$\sum_{i=1}^{5} \langle A_i \rangle = \sum_{a_1,a_2,a_3,a_4,a_5} p(A_1 = a_1, \ldots, A_5 = a_5)(a_1 + a_2 + a_3 + a_4 + a_5) \leq 2.$$

Here, the bound of 2 follows because in each run the maximum value of the sum of the outcomes, $a_1 + a_2 + a_3 + a_4 + a_5$ is 2. Therefore, the KCBS inequality (5.2) follows from the existence of the joint probability distribution in any non-contextual theory.

Let us now follow an alternative information-theoretic approach to deriving a non-contextual inequality using the five-cycle. Assume that despite the fact that not all five projectors are jointly measurable, there exists a joint probability distribution $p(A_1, \ldots, A_5)$. This joint probability distribution is a non-contextual description of the measurements in the set $\{A_i\}$. It is then possible to define the joint entropy $H(A_1, A_2, A_3, A_4, A_5)$, where $H(A) = -\sum_a p(A = a) \log_2 p(A = a)$ denotes the Shannon entropy. Two classical properties of the Shannon entropy will be used in the derivation of the entropic non-contextual inequality. The first is the chain rule $H(A, B) = H(A|B) + H(B)$ and the second is $H(A|B) \leq H(A) \leq H(A, B)$. The latter inequality has the intuitive interpretation that conditioning cannot increase information content of a random variable A and that two random variables A, B cannot contain less information than one of them. Repeated application of the chain rule to the joint entropy $H(A_1, A_2, A_3, A_4, A_5)$ yields

$$\begin{aligned} H(A_1, A_2, A_3, A_4, A_5) &= H(A_1|A_2, A_3, A_4, A_5) + H(A_2|A_3, A_4, A_5) \\ &\quad + H(A_3|A_4, A_5) + H(A_4|A_5) + H(A_5). \end{aligned}$$

Using the inequalities $H(A_1) \leq H(A_1, \ldots, A_5)$ and $H(A_i|A_{i+1}, \ldots, A_5) \leq H(A_i|A_{i+1})$ for

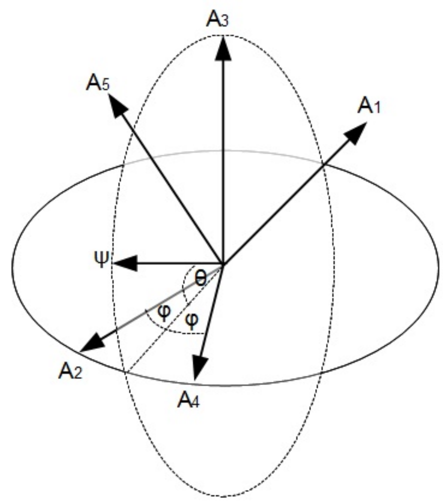

Figure 5.5: Configuration of projectors $\{A_1, \ldots, A_5\}$ leading to maximal violation of the entropic contextual inequality by the state ψ of a three-level system.

$i \in \{1, 2, 3\}$, one then obtains the entropic non-contextual inequality

$$H(A_1|A_5) \leq H(A_1|A_2) + H(A_2|A_3) + H(A_3|A_4) + H(A_4|A_5). \tag{5.3}$$

It is important to notice that all entropies in the above inequality can be evaluated within quantum theory since they refer to jointly measurable quantities. The inequality (5.3) is qualitatively and quantitatively different from the KCBS-type inequality (5.2). We now study the configuration of projectors leading to the optimal violation of the entropic inequality in a three-level quantum system.

For the three-level system the maximal violation of this inequality can be derived to be of magnitude 0.091 bits. The optimal solution can be written with parameters $\theta = 0.2366$ and $\varphi = 0.1698$ (see Fig.(5.5) and Fig.(5.6))

$$|\psi\rangle = \begin{pmatrix} \sin\theta \\ \cos\theta \\ 0 \end{pmatrix}, \quad |A_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{\sqrt{\cos 2\varphi}}{\cos\varphi} \\ \tan\varphi \\ 1 \end{pmatrix},$$

$$|A_2\rangle = \begin{pmatrix} 0 \\ \cos\varphi \\ -\sin\varphi \end{pmatrix}, \quad |A_3\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},$$

$$|A_4\rangle = \begin{pmatrix} 0 \\ \cos\varphi \\ \sin\varphi \end{pmatrix}, \quad |A_5\rangle = \frac{|A_1\rangle \times |A_4\rangle}{||\ |A_1\rangle \times |A_4\rangle\ ||},$$

where $\times$ denotes the three-dimensional vector product. Note from Fig.(5.5) that $|A_1\rangle$

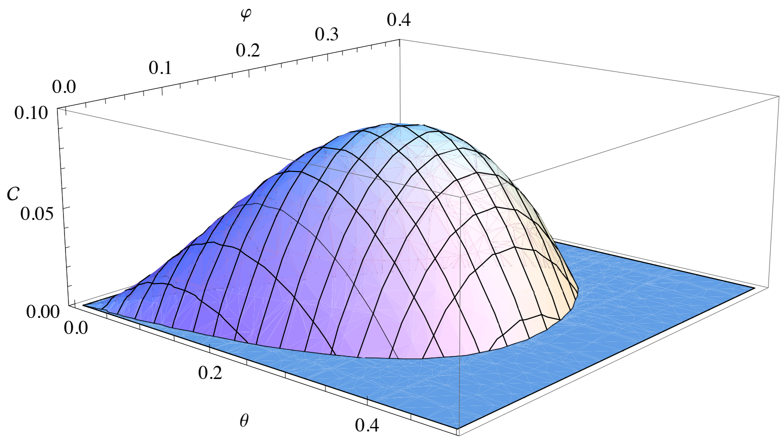

Figure 5.6: Maximal violation of the entropic contextual inequality plotted as a function of the parameters θ and ϕ is seen to be 0.091 bits.

and $|A_5\rangle$ in addition to orthogonality obey the symmetries (i) $\langle A_5|\psi\rangle = \langle A_1|\psi\rangle$, (ii) $\langle A_5|A_2\rangle = \langle A_1|A_4\rangle$ and (iii) $\langle A_5|A_3\rangle = \langle A_1|A_3\rangle$. These symmetries uniquely define $|A_1\rangle$ and $|A_5\rangle$. The maximal violation can be seen to be 0.091 bits in Fig. (5.6), where the violation of the inequality has been plotted as a function of the parameters θ and ϕ.

The intuitive reason for the appearance of these symmetries in the optimal solution is the following. Maximal violation of the entropic contextual inequality requires maximizing $H(A_1|A_5)$ while simultaneously minimizing terms on the right side of the inequality. For orthogonal projectors A and B

$$H(A|B) = p(B=0)H(A|B=0),$$

since $B = 1$ necessarily implies that $p(A = 0) = 1$ so that the entropy of that outcome is zero. If A, B and the state $|\psi\rangle$ are coplanar, $p(A = 1) + p(B = 1) = 1$. This implies that $H(A|B = 0) = 0$ because $p(A = 0) = p(B = 1)$ and $p(A = 1) = p(B = 0)$. Therefore, we need to set all pairs of projectors corresponding to terms on the right-hand side of the inequality as coplanar with $|\psi\rangle$ as possible, while at the same time maximizing $H(A_1|A_5)$. The symmetries listed above arise as a consequence of this consideration. Numerical optimization over the five projectors and the state also reveals these symmetries for the solution. Note that any pure state of a three-level system violates inequality (5.3), the optimal projectors being obtained from the above solution by appropriate Euler rotations from the configuration in Fig. (5.5).

Although the entropic inequality constructed here involves five projectors as in the KCBS inequality (5.2), it is not equivalent to the pentagram inequality constructed there. For the KCBS pentagram inequality, violation is obtained if and only if the joint probability distribution does not exist. However, while violation of the entropic non-contextual inequality (5.3) implies violation of the pentagram inequality, the converse is not true. Moreover, the optimal projectors for violation of (5.3) do not possess the symmetry of the projectors in the pentagram inequality. For the optimal projectors and the state given above, the violation of the pentagram inequality has magnitude 0.049 which is less than the maximal violation of $\sqrt{5}-2$. The pentagram inequality has been tested in the laboratory in [99], a similar setup can be used to test the entropic inequality as well. One advantage of the entropic non-contextual inequalities is that they can be easily constructed for more projectors than five and applied to higher dimensional quantum systems by simply following a similar construction to the one above.

Since these inequalities are not equivalent to those following from the approach in [98], an interesting open question is to investigate the set of quantum states that violate entropic non-contextual inequalities as opposed to the set that violates the KCBS-type inequalities. The approach there is based on studying the extremal edges of a polyhedral cone, which leads to a finite set of inequalities that are in general hard to construct and interpret. Entropic non-contextual inequalities are simpler to construct and carry a clear information-theoretic interpretation. The violation of the entropic non-contextual inequality indicates that the joint probability distribution does not exist. Insistence on a joint probability distribution would result in negative information whose deficit is measured by the violation of the inequality. Moreover, for a single three-level system no entanglement exists and therefore violation of the entropic inequality is solely due to contextuality, unlike the entropic Bell inequality in [100] where entanglement was necessary. Another open question is to study how these inequalities extend to macroscopic systems where entropies arise naturally in statistical mechanics.

5.2 Monogamy of contextuality

As seen in a previous chapter, quantum correlations as captured by the violation of Bell inequalities obey the interesting and useful property of monogamy [58]; if Alice is able to violate a Bell inequality with Bob, she is unable to violate the same Bell inequality with Charlie. Let us reiterate though that this property only arises under certain conditions, namely: i) Alice uses the same settings to violate Bell inequalities with both Bob and Charlie; ii) No communication between Alice, Bob and Charlie is allowed; iii) Bob and Charlie cannot use more measurement settings than two; iv) Alice tries to violate the very same Bell inequality with both Bob and Charlie. Bell monogamies in addition to being useful in secure quantum key distribution [56], interactive proof systems [44] etc. were also seen to behind the emergence of a local realistic description for correlations in the macroscopic domain.

The fact that the origin of Bell inequalities and non-contextual inequalities is the same, namely the existence of a joint probability distribution, suggests that a similar monogamy relation may hold for non-contextual inequalities as well. Bell monogamy arises as a consequence of the principle of no-signaling, which states that the probabilities of outcomes of measurement in one subsystem are independent of the choice of measurement in a spatially separated subsystem. An interesting question which we now proceed to investigate is how the properties of no-signaling and monogamy translate to non-contextual inequalities. In this section, we focus on entropic and KCBS-type non-contextual inequalities and show that there is a form of monogamy of their violations analogous to the monogamy of Bell inequality violations. To do this, we exploit the principle of no-disturbance that is a generalization of the principle of no-signaling.

Gleason Principle of no-disturbance. To formulate the principle of no-disturbance mathematically, let us consider a physical system on which one can perform several different measurements A, B, C, etc. Let us assume that measurements A and B can be jointly performed as can measurements A and C. This implies the existence of the joint probabilities $p(A = a, B = b)$ and $p(A = a, C = c)$ (where as before, small letters denote outcomes of the measurements which are denoted by capital letters). The principle of no-disturbance then stipulates that the marginal probability $p(A = a)$ calculated from $p(A = a, B = b)$ is the same as that calculated from $p(A = a, C = c)$, i.e.,

$$\sum_b p(A = a, B = b) = \sum_c p(A = a, C = c) = p(A = a). \tag{5.4}$$

This property has been referred to as the Gleason property [102] since it is the condition underlying Gleason's theorem. Note that when measurements B, C are performed on spatially separated systems the principle of no-disturbance is exactly that of no-signaling. In this section, again for notational convenience we use $p(A = a, B = b)$ and $p(a, b)$ interchangeably wherever there is no possibility of confusion.

Monogamy of KCBS-type inequalities We concentrate first on the KCBS inequality (5.2) and construct a monogamy relation for it. Similar monogamies hold for any inequalities such as the entropic inequality formulated in the previous section. Let us first rewrite the KCBS inequality as

$$\sum_{i=1}^{5} p(A_i = 1) \leq 2, \tag{5.5}$$

where again A_i are projective measurements with outcomes $a_i = 0, 1$.

Recall that these measurements are cyclically compatible, i.e., it is possible to experimentally determine $p(a_i, a_{i+1})$ (where addition is modulo 5), exclusive ($a_i a_{i+1} = 0$), and can be represented by the commutation graph corresponding to a pentagon Fig.(5.4). Now let us derive a monogamy relation for the above non-contextual inequality from the no-disturbance principle, along similar lines to the monogamy of Bell inequality violations derived from the no-signaling principle [58]. Consider two sets of cyclically compatible and exclusive measurements $\{A_i\}$ and $\{A'_i\}$. Each set gives rise to a KCBS inequality (5.5).

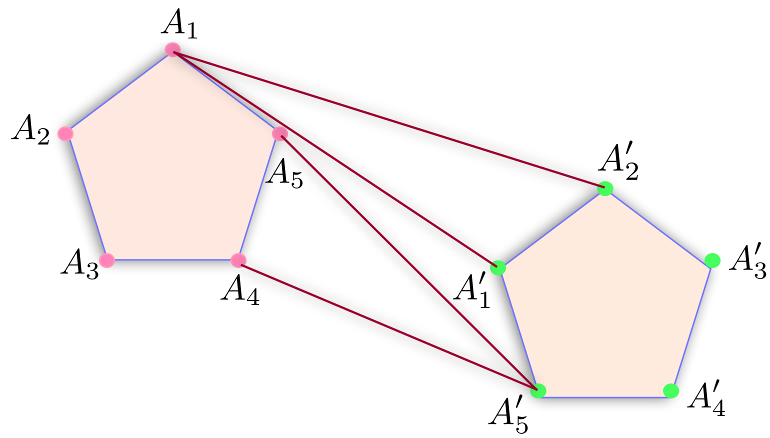

Figure 5.7: Graphical representation of two KCBS inequalities that satisfy the monogamy relation.

Let us assume that the triple A_1, A'_1, A'_2 are jointly measurable and mutually exclusive, as is also the triple A_4, A_5, A'_5. This scenario is represented by the commutation graph in Fig.(5.7). Therefore, in addition to $p(a_i, a_{i+1})$ and $p(a'_i, a'_{i+1})$, one can experimentally determine probabilities $p(a_1, a'_1, a'_2)$ and $p(a'_5, a_4, a_5)$. This condition is similar to a condition imposed in the derivation of Bell monogamies, namely that the common observer Alice chooses the same settings for the violation of Bell inequalities with the other observers Bob and Charlie.

Now we introduce the no-disturbance principle (5.4) by setting $p(A_1 = 1) = p$ and $p(A'_5 = 1) = q$. Mutual exclusiveness then implies that $p(A'_1 = 1) + p(A'_2 = 1) \leq 1 - p$ and $p(A_4 = 1) + p(A_5 = 1) \leq 1 - q$ in addition to $p(A_i = 1) + p(A_{i+1} = 1) \leq 1$ and $p(A'_i = 1) + p(A'_{i+1} = 1) \leq 1$. This in turn implies that $\sum_{i=1}^{5} p(A_i = 1) \leq 2 - q + p$ and $\sum_{i=1}^{5} p(A'_i = 1) \leq 2 - p + q$ and therefore the monogamy relation

$$\sum_{i=1}^{5} p(A_i = 1) + \sum_{i=1}^{5} p(A'_i = 1) \leq 4 \tag{5.6}$$

holds. Therefore, only one KCBS inequality out of the two sets $\{A_i\}$ and $\{A'_i\}$ can be violated in all theories that obey the no-disturbance principle, in particular in quantum mechanics.

If however the principle of no-disturbance does not hold, it is possible to violate both inequalities simultaneously. This is because in this case $p(a_1)$ calculated from $p(a_1, a'_1, a'_2)$ could yield a different value than that calculated from $p(a_1, a_5)$ or $p(a_1, a_2)$ (similarly for A'_5). The consequence of this would be that causality is violated, as can be seen from the following argument. In order to evaluate probabilities, joint measurements do not have to be performed simultaneously, they may also be performed in sequential order. The fact that $p(a_1)$ depends on whether A_1 was measured with A'_1, A'_2 or with A_2 or A_5 can then be used to signal backward in time. The marginal probabilities $p(a_1)$ calculated from $p(a_1, a'_1, a'_2)$ being not consistent with the probability $p(a_1)$ measured earlier (in a joint measurement of A_1 and A_2 for instance) would imply an influence propagating backward in time, thus violating causality [81]. The no-signaling principle being a special instance of the no-disturbance principle, violation of no-signaling monogamy for Bell inequalities implies the possibility of superluminal communication between spatially separated systems, and also leads to a violation of causality. In fact, the method used above for the derivation of monogamies of non-contextual inequalities from the no-disturbance principle can be recognized to be exactly the one used in a previous chapter for the derivation of monogamies of Bell inequality violations from the no-signaling principle.

We have seen an instance of a monogamy relation for non-contextual inequalities, let us now proceed to precisely formulate the method for deriving monogamies for non-contextual (and Bell) inequalities. Given a commutation graph representing a set of n non-contextual inequalities, we look for its vertex decomposition into m chordal subgraphs (each of which admits a joint probability distribution by the Proposition 1), such that the sum of the non-contextual bounds (independence numbers) of these subgraphs is $n \times R$. All vertices of the commutation graph are to be included in the vertex decomposition into subgraphs with no vertex appearing in more than one subgraph, but the edges between the different subgraphs can be neglected. Note that while many non-contextual inequalities involve rank-1 projectors, where the edges of the graph denote mutual exclusiveness in addition to compatibility, this assumption is not crucial to the derivation of monogamies. This can be seen in the derivation of the Bell inequality monogamies where compatibility alone is available and required.

Using the method presented above, one can identify several commutation graphs that yield contextual monogamy (and Bell monogamy) relations, for instance the monogamy relation (5.6) also holds for the graphs in Fig. 5.8(a) and Fig. 5.8(b) as can be seen by the vertex decompositions shown in the figure. We see that monogamy relations for two KCBS inequalities can be derived for various measurement configurations, the measurement configuration given in Fig. 5.7 being the minimal one (with fewest edges connecting two contextual graphs) in which such monogamies appear for two sets of five distinct measurements. This minimality can be seen by finding that for all graphs with one, two and three edges connecting two distinct pentagon graphs, no vertex decomposition into two or more chordal subgraphs with total independence number 4 exists. Since the KCBS inequality (5.5) is a necessary and sufficient condition for the existence of non-contextual description for the five measurements, the relation (5.6) holds for any non-contextual inequality of this kind as well such as the entropic inequality formulated previously. The method can also be used to construct monogamy relations for inequalities with more than

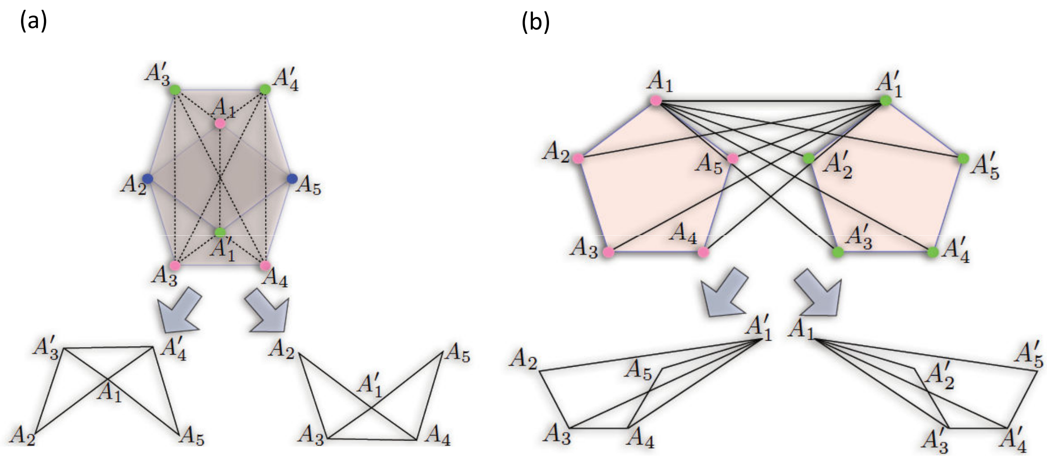

Figure 5.8: Measurement configurations (top) and their vertex decompositions (bottom) for which monogamy relations can be derived.

five measurements along similar lines. In general, it can be seen that the larger the number of mutually exclusive and jointly performable measurements, the stronger the monogamy relation is.

We now proceed to explicitly identify the commutation graphs that lead to monogamy relations for a given set of n KCBS-type non-contextual inequalities (with non-contextual bound R). This is done in the Proposition 2 which provides the necessary and sufficient condition for a commutation graph to give rise to a monogamy relation using the method outlined above. The proof technique can also be easily extended to apply to monogamies for a number of non-contextual inequalities that do not all have the same bound.

We first establish some graph theoretic terminology. As stated before, the independence number $\alpha(G)$ of a graph G is the size of the largest independent set of G, where an independent set is a set of vertices of which no pair is adjacent (joined by an edge). The vertex clique cover number $\bar{\chi}(G)$ is the minimal number of cliques needed to cover all the vertices of the graph, a clique denoting a fully connected subgraph. The clique number $\omega(G)$ is the size of the largest clique contained in the graph. The chromatic number $\chi(G)$ is the minimum number of colors needed to properly color all the vertices of G where no two adjacent vertices have the same color. The complement of a graph G is a graph $\bar{G}$ on the same set of vertices such that any two vertices in $\bar{G}$ are adjacent if and only if they are non-adjacent in G. Finally, a perfect graph is a graph G which has the property that $\omega(G') = \chi(G')$ for all induced subgraphs G' of G. We are now ready to formally state the condition for a commutation graph to yield monogamy relations.

Proposition 2: Consider a commutation graph G representing a set of n KCBS-type non-contextual inequalities $I_j \leq R$ $(j = 1, ..., n)$ where each inequality has non-contextual bound R. Then this graph gives rise to a monogamy relation using the outlined method if and only if its vertex clique cover number is $n \times R$.

Proof:

The condition that the vertex clique cover number is $n \times R$ is seen to be sufficient as each clique has an independence number of 1, and cliques are the only graphs with independence number 1. Thus, a vertex decomposition of the commutation graph into n cliques would give rise to the monogamy relation, $\sum_{j=1}^{n} I_j \leq n * R$.

We now show that this condition is also necessary for a commutation graph to result in a monogamy relation by our method. Recall that the method relies on the vertex decomposition of the commutation graph into $m \leq n * R$ chordal subgraphs $(G_1, ..., G_m)$ each of which admits joint probability distribution, such that the sum of their independence numbers is $n \times R$, i.e., $\sum_{j=1}^{m} \alpha(G_i) = n \times R$. Now, all chordal graphs are known to be perfect, i.e., the size of the largest clique in every induced subgraph of the chordal graph equals the number of colors needed to color that induced subgraph [108]. For all perfect graphs G, $\alpha(G)$ can be shown to be equal to $\bar{\chi}(G)$, by the following series of equalities. Note that from the definition of a perfect graph $\omega(G) = \chi(G)$ by taking the induced subgraph of G to be G itself. That is, the size of the largest clique in the graph is the minimum number of colors needed to properly color G. For all perfect graphs G, their complement graph is also perfect by the Weak Perfect Graph Theorem [109], i.e., $\omega(\bar{G}) = \chi(\bar{G})$. It is readily seen that for any graph G, $\omega(\bar{G}) = \alpha(G)$, i.e., the independence number of a graph is equal to the size of the largest clique in its complement graph. Also, it can be seen that $\chi(\bar{G}) = \bar{\chi}(G)$ as the number of colors required to color a graph G is equal to the number of cliques that cover $\bar{G}$. From the above equalities, the following result is obtained that for all perfect graphs, and in particular for chordal graphs G,

$$\alpha(G) = \bar{\chi}(G), \tag{5.7}$$

i.e., the independence number of a chordal graph is equal to its vertex clique cover number.

Now, by eqn.(5.7), in the derivation of the contextual monogamy relation by vertex decomposition into chordal subgraphs, $\sum_{j=1}^{m} \alpha(G_i) = \sum_{j=1}^{m} \bar{\chi}(G_i) = n \times R$. That is, the chordal subgraphs can be vertex decomposed further exactly into a set of $n \times R$ cliques. This proves that the condition that the vertex clique cover number be equal to $n \times R$ is both necessary and sufficient for a commutation graph to result in a contextual monogamy relation by the method outlined. This ends the proof.

The above necessary and sufficient condition gives a very powerful method of identifying whether a given graph exhibits contextual monogamy by finding its vertex clique cover number to check if it is equal to $n \times R$. If we have a set of n non-contextual inequalities such that n_1 of them have a bound of R_1, n_2 of them have a bound of R_2, and in general n_k of them have a bound of R_k, then it is easy to see that the proof extends to give the necessary and sufficient condition as the vertex clique cover number being equal to $\sum_j n_j R_j$, i.e., $\bar{\chi}(G) = \sum_j n_j R_j$. Note that we are not interested in the case that $\bar{\chi}(G) < n * R$ since as we shall see below, this gives rise to monogamies even within classical non-contextual theories.

The monogamy relations presented so far are genuine properties of contextual theories in the sense that for classical (non-contextual) theories each of the two inequalities can achieve its maximal value within the non-contextual theory. We note, however, that certain monogamies also hold for non-contextual theories, for instance for the situation when all measurements in set $\{A_i\}$ are compatible and mutually exclusive with all the measurements in set $\{A'_i\}$. Here the mutual exclusiveness guarantees the monogamy $\sum_{i=1}^{5} p(A_i = 1) + \sum_{i=1}^{5} p(A'_i = 1) \leq 5/2$ in all theories obeying the no-disturbance principle. However, an important feature here is that monogamies also arise within non-contextual theories for which the relation $\sum_{i=1}^{5} p(A_i = 1) + \sum_{i=1}^{5} p(A'_i = 1) \leq 2$ holds so that both the inequalities cannot achieve their non-contextual bound of 2 simultaneously. This can be traced to the large number of mutually exclusive measurements required here. The interesting monogamies are those in which such classical restrictions do not appear such as those in Fig.(5.7) and Fig.(5.8).

Let us now show how the monogamy relation (5.6) applies within quantum theory. Firstly, note that measurements for the optimal violation of KCBS inequality for a single three-level quantum system are rank-1 projectors spanning real three-dimensional space. Consider a real four-dimensional space in which the set of projectors $\{A_i\}$ spans dimensions $1, 2$ and 3 and the set of projectors $\{A'_i\}$ spans dimensions $2, 3$ and 4. These projectors can be constructed to obey the constraints of mutual exclusiveness and joint measurability as required by the commutation graphs. For example, a set of projectors that correspond to the measurement configuration in Fig. 5.8(b) for a quantum mechanical system of dimension four is given by

$$
\begin{aligned}
|A_1\rangle &= (1,0,0,0)^T,\ |A_2\rangle = (0,1,0,0)^T,\\
|A_3\rangle &= (\cos\theta, 0, \sin\theta, 0)^T,\\
|A_4\rangle &= (\sin\alpha\sin\theta, \cos\alpha, -\sin\alpha\cos\theta, 0)^T\\
|A_5\rangle &= \frac{1}{\sqrt{\cos^2\alpha + \sin^2\alpha\cos^2\theta}}(0, \sin\alpha\cos\theta, \cos\alpha, 0)^T,\\
|A'_1\rangle &= (0,0,0,1)^T,\quad |A'_2\rangle = (0, \cos\beta, \sin\beta, 0)^T,\\
|A'_3\rangle &= (0, \sin\gamma\sin\beta, -\sin\gamma\cos\beta, \cos\gamma)^T,\\
|A'_4\rangle &= (0, \sin\delta\sin\varepsilon, -\sin\delta\cos\varepsilon, \cos\delta)^T,\\
|A'_5\rangle &= \frac{1}{\sin\delta}(0, \sin\delta\cos\varepsilon, \sin\delta\sin\varepsilon, 0)^T,
\end{aligned}
\tag{5.8}
$$

where we impose the conditions $\sin(\beta-\varepsilon) \neq 0$, $\cos(\beta-\varepsilon) \neq 0$ and $\tan\delta\tan\gamma\cos(\beta-\varepsilon) = -1$. This is analogous to the situation where one requires three qubits (dimension 8) which is the minimal system in order to observe monogamy of Bell inequality violations. Since quantum theory obeys the principle of no-disturbance, the monogamy inequality (5.6) is guaranteed to hold for these projectors. However, quantum mechanics incorporates other properties as well such as the complementarity principle. For the monogamy relations of Bell inequalities, the exact trade-offs between multiple inequalities within quantum theory were derived using the principle of correlation complementarity. An important open problem is to derive the exact trade-offs for non-contextual inequalities within quantum theory over and above those imposed by the no-disturbance principle.

Violation of a single non-contextual inequality (5.5) for a three-level system has been experimentally tested using a single photon [99]. The monogamy of contextuality presented here can be realized for a four-level system with feasible modifications to the existing experimental setup, and using projectors according to the identified commutation graphs. This would establish the monogamy of contextuality as a distinct phenomenon from the monogamy of entanglement, since the notion of entanglement is not clearly applicable to a single quantum system. The fact that Bell inequalities and non-contextual inequalities arise from the same origin leads one to believe that features seen in the Bell scenario should carry over to the contextual scenario as well. In this regard, interesting open projects concern the investigation of how other features such as distillation, activation of non-locality, no-signaling boxes (or Popescu-Rohrlich boxes) [110, 102] and information causality [68] carry over to the contextual scenario.

Chapter 6

Macroscopic Non-Contextuality

We have seen in a previous chapter that for the measurements that can be feasibly performed on a macroscopic system, a local realistic description of the correlations can be found. Indeed, we were able to construct an explicit local realistic model for such correlations. We have since seen that contextuality is arguably a more general notion than local realism, revealing aspects of realism in single systems without the constraint of locality and that all quantum systems of dimension greater than two are known to be contextual by the Kochen-Specker theorem. We might therefore reasonably ask whether macroscopic systems can be shown to be contextual if we are restricted to the feasible measurements that can be performed on these systems. Contextuality being a significant aspect of quantum theory distinguishing it from non-contextual classical theories, this question merits a detailed investigation which we shall proceed to carry out in this chapter.

Our everyday observation of the macroscopic world supports the assumption of non-contextuality while quantum theory portrays a picture of the world devoid of this notion. The arguments used by Bell and Kochen-Specker are the basis of experimentally verifiable criteria for identifying certain physical phenomena that cannot be explained by any non-contextual theory [41, 98]. These criteria are given as a violation of certain inequalities, which we called non-contextual inequalities; indeed for microscopic systems such as a single photon [99] or a pair of photons [52], it has been experimentally proven that these non-contextual inequalities are violated. These inequalities require measurements that can be performed in different contexts (hence their name); to show that quantum theory is a contextual theory, i.e., it does not allow for a joint probability distribution, one needs multiple contexts [9].

Moreover, to apply non-contextual inequalities to a quantum system, both commuting and non-commuting observables are required. If only commuting observables $\{A_1, \ldots, A_N\}$ say, were available, the joint probability distribution is given within quantum mechanics as $p(A_1 = a_1, \ldots, A_N = a_N) = tr(\rho P_{a_1}^{A_1} \otimes \cdots \otimes P_{a_N}^{A_N})$, where ρ is the state of our quantum system and $P_{a_k}^{A_k}$ refers to the projector onto the subspace corresponding to the value a_k for the observable A_k. For example, for a spin-1/2 system, the projectors corresponding to the measurements up along z direction $P_+^z = |\uparrow_z\rangle\langle\uparrow_z|$ and down along the z direction $P_-^z = |\downarrow_z\rangle\langle\downarrow_z|$ can be seen to commute (these projectors are orthogonal). If only non-commuting observables $\{A_1, \dots, A_N\}$ were available, the joint probability distribution does not exist within quantum theory. However, a hypothetical joint probability distribution can be constructed as $p(A_1 = a_1, \dots, A_N = a_N) = p(A_1 = a_1)p(A_2 = a_2)\dots p(A_N = a_N)$. This distribution recovers all the measurable probabilities as marginals $p(A_k = a_k) = \sum_{\{a_i\}, i\neq k} p(A_1 = a_1, \dots, A_N = a_N)$. Since no two observables commute in this scenario, no contexts exist and no other marginals can be measured experimentally. Hence, we see that in order to observe a macroscopic violation of contextual inequalities, we require both commuting and non-commuting observables and moreover, these observables are required to be macroscopically feasible.

In this chapter, we study a many-body system of spins of an arbitrary dimension and consider experimentally feasible measurements, such as magnetization. We show that non-contextual inequalities or Kochen-Specker proofs cannot be constructed from macroscopic measurements by proving that the projectors of these measurements along non-parallel directions do not commute, hence one cannot find contexts. This would imply that the question of macroscopic quantum contextuality is experimentally undecidable, i.e., collective behaviors of a many-body quantum system can be described using classical (non-contextual) or quantum (contextual) theories. However, we shall see that there remain certain experimental possibilities of creating contexts in these systems for which it remains an open question whether non-contextual inequalities constructed using macroscopic measurements can be violated by quantum states. We also note that if one considers coarse-grained measurements, then it has been shown [84] that again a non-contextual description emerges for macroscopic systems. The proof that no contexts can be found in sharp macroscopic magnetization measurements is a detailed version of that presented in [111], however new material regarding possible realizations of contexts is also included here.

6.1 Feasible macroscopic measurements

Let us first recapitulate the main ideas in the notion of feasible measurements on macroscopic systems. For simplicity, let us consider a magnetic system consisting of N spin-s particles. When the number of spins becomes large ($N \approx 10^{23}$), feasible measurements are limited to measurements of magnetization in some direction $\vec{n}$. These are given by a set of projectors of the form

$$\mathbb{P}_m(\vec{n}) = \sum_{k_1+\cdots+k_N=m} \mathbb{P}_{k_1}(\vec{n}) \otimes \cdots \otimes \mathbb{P}_{k_N}(\vec{n}), \tag{6.1}$$

where each $k_i = -s, -s+1, \dots s$ and m corresponds to different degrees of magnetization. This limitation on the set of measurements that can be performed is imposed despite the generalized spin measurement proposal in [112] by the following two factors.

The first restriction is imposed by the fact that a physical description for a system consisting of a large number of particles N is best done by statistical theories. The basic assumption in these theories is that one cannot know the exact micro-state of the system and is hence forced to assume *a priori* that all micro-states leading to the same macro-state are equally probable. Indeed, this assumption goes by the name of equal a priori probabilities in statistical mechanics and is used in the description of these systems by the micro-canonical, canonical or grand canonical ensembles. One of the consequences of this assumption is that any observable that can be measured does not distinguish between micro-states having the same macroscopic property. All states corresponding to a given property belong to a permutationally invariant subspace, this in turn implies effective indistinguishability of the particles and yields the form of the projectors in equation (6.1). We stress that this indistinguishability is not due to the fundamental indistinguishable particles of quantum theory, namely fermions and bosons, but rather is brought about by the permutational invariance of our macroscopic measurements. The permutational invariance of the projectors is therefore a key feature of feasible measurements on any macroscopic system.

The second restriction is due to the fact that, for spin systems, magnetization dominates more exotic multipole moments. In principle it is possible to measure the k-pole moment of magnetization for a spin-s particle, where $k \leq 2s+1$ [112]. Therefore, there is no theoretical limitation to measuring a macroscopic k-pole observable that, analogous to magnetization, is a sum of k-pole moments of all spins in the system. However, the electromagnetic fields required for measuring the k-pole moments are infeasible to implement in practice. Moreover, higher moments such as susceptibility are not suitable observables to study contextuality as they deal with states that are varying in time. Hence, the feasible measurements to study contextuality of macroscopic spin systems are restricted to magnetization.

6.2 Lack of contexts in macroscopic measurements

We now show that under the above restrictions there is no context for macroscopic measurements of magnetization along two directions $\vec{n}$ and $\vec{n}'$, namely, $[\mathbb{P}_m(\vec{n}), \mathbb{P}_n(\vec{n}')] = 0$ if and only if $\vec{n} = \pm\vec{n}'$.

A simple graphical illustration of the above fact is shown in Fig. (6.1) which depicts a graphical representation of the spin-1 (the smallest contextual system) states along two different directions $\vec{n}$ and $\vec{n}'$. Spin-1 can be represented as a vector of length $\sqrt{2}$ in three dimensional space and has three values along any measurement direction $\{+1, 0, -1\}$,

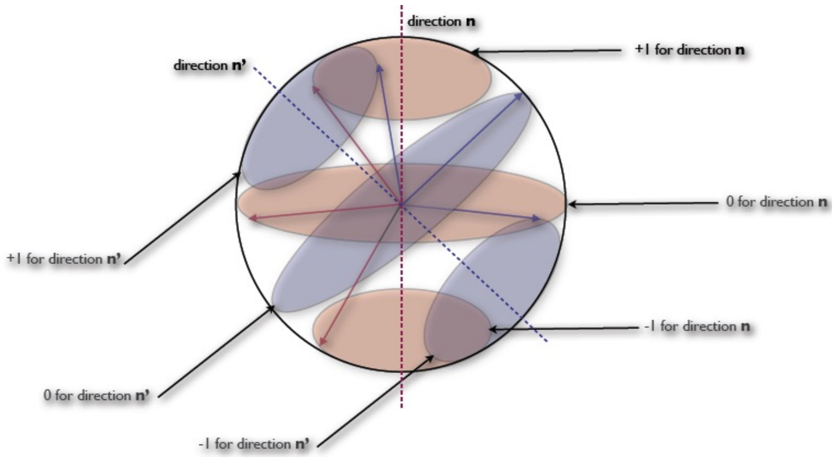

Figure 6.1: Graphical illustration of the spin-1 system. Horizontal (red) circles depict the projectors $\mathbb{P}_{-1}(\vec{n}), \mathbb{P}_0(\vec{n}), \mathbb{P}_{+1}(\vec{n})$ and slant (blue) ones depict $\mathbb{P}_{-1}(\vec{n}'), \mathbb{P}_0(\vec{n}'), \mathbb{P}_{+1}(\vec{n}')$. Projectors for $+1, 0, -1$ outcomes along different directions $\vec{n}$ and $\vec{n}'$ commute only if the two vectors are parallel.

therefore we have three arrows per direction. Due to the Heisenberg uncertainty only one coordinate of the spin vector can be determined, namely the one along the measurement direction. The other two coordinates remain undetermined hence for each measurement outcome along direction $\vec{n}$ (or $\vec{n}'$) the tip of the spin vector is spread over the rim of the corresponding circle. Horizontal red circles depict the projectors $\mathbb{P}_{-1}(\vec{n}), \mathbb{P}_0(\vec{n}), \mathbb{P}_{+1}(\vec{n})$ and slant blue ones depict $\mathbb{P}_{-1}(\vec{n}'), \mathbb{P}_0(\vec{n}'), \mathbb{P}_{+1}(\vec{n}')$. It can then be seen graphically that $[\mathbb{P}_m(\vec{n}), \mathbb{P}_{m'}(\vec{n}')] = 0$ if and only if the two vectors are parallel. Similar results will be seen to hold for systems composed of a large number of spins of any dimension.

We now proceed to construct the proof for the general situation and show that there is no context for macroscopic measurements of magnetization along two directions $\vec{n}$ and $\vec{n}'$. Without loss of generality we may assume $\vec{n}$ defines the Z axis and that $\vec{n}'$ lies on the XZ plane. We denote the projectors corresponding to the magnetization measurement along the Z axis with the eigenvalue m by $\mathbb{P}_m$. The projectors of the second measurement are denoted by $\tilde{\mathbb{P}}_n$ and are related to $\mathbb{P}_m$ via rotation operator $\mathcal{D}(\beta)$, i.e., $\tilde{\mathbb{P}}_n = \mathcal{D}(\beta)\mathbb{P}_m\mathcal{D}^\dagger(\beta)$.

Since we are dealing with $N \gg 1$ particles, there are two different representations of $\mathbb{P}_m$. The first one is given via the tensor product of spin states corresponding to different particles

$$\mathbb{P}_m = \sum_{k_1+\cdots+k_N=m} \left(|k_1\rangle \otimes \cdots \otimes |k_N\rangle\right)\left(\langle k_1| \otimes \cdots \otimes \langle k_N|\right),$$

whereas the second is given via a direct sum of spin states corresponding to different values of total angular momentum

$$\mathbb{P}_m = \sum_{j,\lambda_j} |j,\lambda_j,m\rangle\langle j,\lambda_j,m|, \tag{6.2}$$

where j runs over all values allowed by standard angular momentum addition rules and λ_j denotes the degeneracy of j, i.e., the number of different realizations of spin j with N particles. Note that $N \gg 1$ leads to a high degeneracy of $\mathbb{P}_m$ and as a result guarantees that the sum in (6.2) runs over many different values of j.

The general form of the rotation matrix (often referred to as the Wigner D-matrix) with coefficients $d^{j,\lambda_j}_{\tilde{m},m}$ can be written as

$$\mathcal{D}(\beta) = \sum_{j,\lambda_j,m,\tilde{m}} d^{j,\lambda_j}_{\tilde{m},m}(\beta)|j,\lambda_j,\tilde{m}\rangle\langle j,\lambda_j,m|.$$

It follows that

$$\tilde{\mathbb{P}}_n = \sum_{j,\lambda_j,\tilde{m},\tilde{m}'} d^{j,\lambda_j}_{\tilde{m},n}(\beta) d^{j,\lambda_j}_{\tilde{m}',n}(\beta)|j,\lambda_j,\tilde{m}\rangle\langle j,\lambda_j,\tilde{m}'|,$$

and

$$[\mathbb{P}_m,\tilde{\mathbb{P}}_n] = \sum_{j,\lambda_j,\tilde{m}} d^{j,\lambda_j}_{m,n}(\beta) d^{j,\lambda_j}_{\tilde{m},n}(\beta) \left(|j,\lambda_j,m\rangle\langle j,\lambda_j,\tilde{m}| - |j,\lambda_j,\tilde{m}\rangle\langle j,\lambda_j,m|\right).$$

The above commutator equals zero if all terms of the corresponding matrix vanish. Let us define

$$\Gamma^{j,\lambda_j}_{k,k'} = \langle j,\lambda_j,k|[\mathbb{P}_m,\tilde{\mathbb{P}}_n]|j,\lambda_j,k'\rangle.$$

In the above we do not consider off-diagonal terms corresponding to different j's and λ's, since they are trivially equal to zero. One easily finds

$$\Gamma^{j,\lambda_j}_{k,k'} = d^{j,\lambda_j}_{m,n}(\beta)\left(\delta_{k,m} d^{j,\lambda_j}_{k',n}(\beta) - \delta_{k',m} d^{j,\lambda_j}_{k,n}(\beta)\right).$$

The commutator vanishes if $\Gamma^{j,\lambda_j}_{k,k'} = 0$ for all allowed j,λ_j,k,k'. Since there is no dependency on λ_j, from now on we skip this superscript. Below we show that there always exists a set of j,k,k' for which $\Gamma^{j}_{k,k'} \neq 0$. First, let us note that $\Gamma^{j}_{k,k'}$ can be nonzero only for $k=m$ and $k' \neq m$, or for $k \neq m$ and $k'=m$. Without losing generality, it is enough to show that there exist j and $k \neq m$ for which

$$d^{j}_{m,n}(\beta) d^{j}_{k,n}(\beta) \neq 0.$$

At this stage let us write explicitly

$$\begin{aligned} d^j_{m',m}(\beta) &= \sqrt{\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!}} \left(\cos\frac{\beta}{2}\right)^{-m-m'} \left(\sin\frac{\beta}{2}\right)^{2j+m+m'} (-1)^{j+m'} \\ &\times \sum_\nu \left((-1)^\nu \binom{j+m}{\nu} \binom{j-m}{j+m'-\nu} \left(\cos\frac{\beta}{2}\right)^{2\nu} \left(\sin\frac{\beta}{2}\right)^{-2\nu} \right), \end{aligned} \tag{6.3}$$

where ν goes over all integer values $\nu \geq 0$ for which the binomial coefficients do not vanish.

We now find conditions under which $d^j_{m',m}(\beta)$ is nonzero. Let us note that in case of two nonparallel magnetization directions ($0 < \beta < \pi$) all trigonometric functions in the above formula are nonzero. Let us consider two cases. First, let us assume that both $m' = m = 0$. In such a case

$$d^j_{0,0}(\beta) = P_j(\cos\beta),$$

where $P_j(x)$ is the Legendre polynomial that obeys

$$\sum_{j=0}^{\infty} P_j(x) t^j = \frac{1}{\sqrt{1 - 2xt + t^2}}, \tag{6.4}$$

and the recursion relation

$$(j+1)P_{j+1}(x) = (2j+1)xP_j(x) - jP_{j-1}(x).$$

We claim that in the allowed range of j for any $-1 < x < 1$ there exists j for which $P_j(x) \neq 0$. Otherwise, the recursion relation would imply that $P_j(x) \neq 0$ for at most a finite set of j, but this is inconsistent with Eq. (6.4), hence it is not possible. Next, consider a case when at least one of labels (m or m') differs from zero. In this case we set $j = \max\{|m|, |m'|\}$ and it is easy to see that the sum in Eq. (6.3) has only one nonzero term.

Finally, let us show that the product of two coefficients $d^j_{m,n}(\beta) d^j_{k,n}(\beta)$ differs from zero. Since in this case j is the same for both coefficients and m and n are fixed, let us again consider two cases. Following the above discussion, if both $m = n = 0$ we set j such that the first coefficient is nonzero and then we set $k = j$. On the other hand, if m or n are nonzero we can guarantee that the first coefficient does not vanish by fixing $j = \max\{|m|, |n|\}$. For the second coefficient note that $k \neq m$. In case $|m| \leq |n|$ it is possible to set k such that $|k| \leq |n|$ and $k \neq m$. Since $j = \max\{|m|, |n|\} = |n|$ both coefficients are nonzero. In case $|m| > |n|$ we set $k = -m$ and $j = \max\{|m|, |n|\} = |m|$, which guarantee that both coefficients are nonzero. This completes the proof that the commutator $[\mathbb{P}_m, \tilde{\mathbb{P}}_n]$ is never zero for two nonparallel magnetization directions.

This implies that under the aforementioned restrictions, contexts cannot be created using macroscopic magnetization measurements. Therefore, these cannot be used to construct any non-contextual inequalities with which to test the non-classicality of macroscopic objects. This sheds more light on one of the most fundamental questions of quantum theory, namely, whether and how realism arises in the macroscopic world although the microscopic constituents of macroscopic objects do not obey realism. If we understand the macroscopic world to possess realism, then we are forced to explain how this realism is created. Yet, we have just seen that we can choose whether to describe the macroscopic world by a theory with realism or by one without; no matter which choice we make, it cannot be refuted since the validity of the choice is experimentally undecidable.

Interestingly, the quantumness of the correlations between composite macroscopic objects is experimentally testable and conforms with local realism. This situation resembles the case of a single qubit versus a pair of qubits. The quantumness of a single qubit is fundamentally undecidable [113, 114] because no contexts can be found for any measurements, whereas the correlations between two qubits are decidable and for entangled states can be shown to be quantum.

6.3 Conclusions and Open Questions

In a sense, we might infer from the considerations above that the restrictions imposed on the set of measurements lead to a simplification of quantum theory that prevents the testability of certain non-intuitive features such as contextuality. On the contrary, other features such as entanglement [87] are still preserved under the same restriction. Similar behavior was observed in a toy model of quantum theory proposed in [115]. An interesting open question is to investigate the complexity of measurements needed for contextuality to emerge in the above scenario. A further question could be to identify the exact trade-off between the size of the system and the complexity of the measurements that can be performed on it.

We conclude this chapter by mentioning one interesting avenue for further research. In spite of the fact that the projectors of magnetization themselves may not yield contexts, one can try to artificially engineer contexts in the system. This can be done by having a set of projectors that commute by virtue of addressing different subsystems within the macroscopic system. One such experimentally possible set up is depicted in Fig.(6.2). In the figure, a macroscopic system of spins is depicted with measurements of magnetization $A_i = \frac{\sum_k n_i^k \cdot \sigma^k}{N_i}$ in five subsystems (denoted by circles forming a pentagram) in the directions n_i $(i = 1, \ldots, 5)$. Here N_i denotes the number of particles in region i, the indices i being ordered as in the pentagram. The magnetization observables in non-overlapping regions commute, i.e. $[A_i, A_{i+1}] = 0$ where we identify A_6 with A_1. One can then construct the KCBS non-contextual inequality using these observables [98]

$$\sum_i \langle A_i A_{i+1} \rangle \geq -3. \tag{6.5}$$

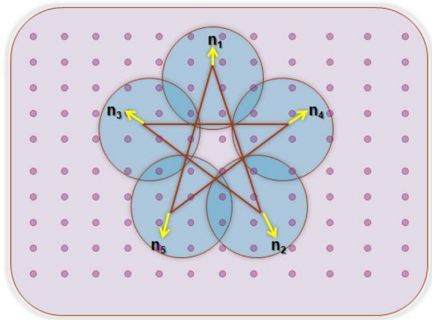

Figure 6.2: A possible scenario in which contexts can be found for macroscopically feasible measurements. Measurements of magnetization $A_i = \frac{\sum_k n_i^k \cdot \sigma^k}{N_i}$ are made on macroscopic subsystems denoted by circles forming a pentagram structure. Using these observables, a KCBS-type contextual inequality can be constructed for the macroscopic system as explained in the text.

As discussed in the previous chapter (where the above inequality was written in terms of projectors taking outcomes 0 or 1), this is the simplest non-contextual inequality for a qutrit. Several such inequalities are known, both in the state-dependent case as above, and also in the state-independent scenario. However, since state-independent inequalities are only known to be violated by all states of *given dimension*, the formulation of such inequalities using magnetization measurements is not a guarantee of macroscopic contextuality. This problem of finding if there exist states which violate non-contextual inequalities such as the above merits further investigation. Numerical results on highly entangled states seem to suggest that no such violation exists, and the open problem is to prove analytically that such a violation is (not) possible.

Another avenue for further research can be described as follows. While we have argued that magnetization and perhaps its moments such as magnetic susceptibility are the only feasible macroscopic measurements, it would also be interesting to consider generalized measurements such as POVM's (Positive Operator Valued Measurements) or weak measurements that do not change the state of the system much. The traditional Kochen-Specker formulation of contextuality requires measurements of the projective type, it remains an open question to show how the information gained about the system from POVM measurements can be used to reveal contextuality [116]. Finally, we note that we may coarse-grain the outcomes of magnetization measurements by grouping together several individual outcomes into one coarse-grained outcome. For these measurements, it has been shown [84] that again a non-contextual description of macroscopic systems emerges. We now turn to our final topic concerning the difference between quantum theory and classical theories, the question of indistinguishable particles, and investigate the relation between this indistinguishability and the correlations in these particles.

Chapter 7

Composite Bosons and Entanglement

Quantum theory incorporates several features that mark its departure from the classical theories of Nature. So far we have investigated some of these such as no-cloning, lack of local realism and contextuality. We now turn to another principal feature of the theory, namely the appearance of identical particles, i.e. particles that are indistinguishable from each other, even in principle. The fundamental particles of Nature can be broadly classified into the two categories of fermions and bosons, according to their group behavior. While any number of bosons can share a quantum state, the Pauli exclusion principle forbids any two indistinguishable fermions from doing so. Most particles in Nature are not elementary, and in fact are composed of elementary fermions or bosons. These composite particles can exhibit a variety of behaviors ranging from fermionic to bosonic depending on the physical situation and the state of the system at hand. In this chapter, we extend our considerations to the correlations in composite particle systems.

Identical particles or indistinguishable particles form an intriguing aspect of quantum theory. In general, macroscopic particles may be distinguished based on their intrinsic properties such as mass, charge or spin. However, microscopic particles such as a group of electrons are completely equivalent in their physical properties; every electron in the Universe has the same properties as every other. A classical method of distinguishing particles is by tracking their trajectories, so that one can distinguish different particles by their spatial position. In quantum theory, the positions of particles between measurements are not fixed. Their wavefunctions that determine the probability of finding them at specified positions may overlap, so that it is impossible to determine which particle was detected in a subsequent measurement. This indistinguishability leads to an additional symmetry in the quantum mechanical description of these particles.

The group behavior of bosons and fermions manifests itself in the quantum wavefunction of these particles. The wavefunction of bosons is symmetric, so that if one boson is in state $|a\rangle$ and an identical boson is in state $|b\rangle$, the wavefunction of the pair is given by the symmetric (un-normalized) form $|a\rangle \otimes |b\rangle + |b\rangle \otimes |a\rangle$. In contrast, the wavefunction of fermions is antisymmetric, so that in an analogous scenario, the wavefunction of a pair of identical fermions would be written $|a\rangle \otimes |b\rangle - |b\rangle \otimes |a\rangle$. This reflects the Pauli exclusion principle, if the two particles were in the same state, say $|a\rangle$, then the wavefunction would be identically zero; in other words, no two identical fermions can occupy the same quantum mechanical state. This at first sight abstract principle is in fact responsible for the chemical properties of atoms, and indeed for the stability of matter itself. When two identical particles are far apart or if they are in separate potential wells so that the overlap of their wavefunctions is negligible, one may distinguish them by means of their position. When they are then brought closer, the wavefunctions are restricted to reside in either the symmetric or antisymmetric Hilbert space, and thus one encounters a reduction in the number of possible states, a property that will be crucial to our considerations later.

The symmetry and antisymmetry has important consequences in the statistical mechanical description of these particles as well. Bosons obey the Bose-Einstein (BE) statistics and fermions obey the Fermi-Dirac (FD) statistics, both of which are different from the Maxwell-Boltzmann statistics of classical distinguishable particles. The BE and FD statistics become particularly prominent in identical particle systems of high densities where there is large overlap of wavefunctions; both statistics are well approximated by the Maxwell-Boltzmann distribution for small densities. We may note that particles with mixed statistics are also possible. For instance, in certain two-dimensional systems, there exist exotic particles known as anyons obeying fractional statistics; evidence for their existence has been found experimentally in the phenomenon of the fractional quantum Hall effect.

The famous spin-statistics theorem by Fierz and Pauli [117] relates the exchange symmetry of the identical particles to their spin. In particular, this theorem states that the wavefunctions of particles with integer spin ($= n\hbar$, with n an integer) must be symmetric under the interchange of the two particles, so that such particles are bosons; and the wavefunctions of particles with half-integer spin ($= \frac{1}{2}(2n-1)\hbar$, with n being an integer) are antisymmetric under exchange, so that such particles are fermions. Particles composed of an even number of fermions (which have half-integer spins) are thus expected to be bosons, and particles containing an odd number of fermions are expected to be fermionic. For example, the hydrogen atom made of one proton and one electron is considered to be a boson and so also is the helium-4 atom containing two protons, two neutrons and two electrons. The fermionic and bosonic behavior of composite particles is the main focus of this chapter. In this regard, it is important to recognize that as per our previous arguments fermionic or bosonic behavior of composite particles is seen at distances larger than the size of the particles. When two composite particles are in close proximity, their constituent structure becomes important. To consider the example of the helium-4 atom, when two such helium-4 atoms are nearby (the separation being of the order of their size which is about an Angstrom, i.e., 10^{-10} m), they cannot share the same space even though the spin-statistics theorem specifies them to be bosons. This is because the Pauli scattering between the constituent fermions becomes significant at short distances and does not allow the constituent particles to share a common state. Thus, the fermionic and bosonic behavior of composite particles is expected to depend on density in addition to their total spin.

In this chapter, we study the "quality of bosonic behavior" of a composite boson made of two distinguishable fermions (such as an exciton, the hydrogen atom, positronium, etc.) and investigate its dependence on the correlations between the two constituent fermions. Our analysis will be based on a simplified model of condensation of the composite particles and tools of quantum information theory such as the majorization criterion for the interconversion between different entangled states via the Local Operations and Classical Communication (LOCC) formalism. We will see that the introduction of these tools yields new insights to the old and important problem of identifying the conditions for the bosonic behavior of these composite bosons. We will precisely identify the role entanglement and its monogamy play in the formation and behavior of such composite particles.

We will then proceed to investigate the general question of identifying the quality of fermionic and bosonic behavior in composite particle systems. Noting that the fundamental processes of single particle addition and subtraction already highlight the differences between fermions, bosons and distinguishable particles, we will construct a measure of fermionic and bosonic quality based on these basic processes. To do so, we utilize the formalism of completely positive maps and Kraus channels as required by the probabilistic nature of these processes. Finally, we will consider another physical situation, namely two-particle interference via a beamsplitter and show that composite particles can display a wide range of behavior from fermionic to bosonic depending on their internal quantum state and the physical situation at hand. The material in this chapter is a detailed account of [118, 119], the LOCC formulation of the toy model of condensation was formulated by the author and collaborators in the first article and the measure of bosonic nature in terms of particle addition and subtraction was proposed in the second.

7.1 Entanglement and composite particle behavior

Let us first introduce the problem following the analysis in [121, **?**]. We begin with the system of a composite boson made of two distinguishable fermions in a pure state. A number of physical systems such as excitons, the hydrogen atom, positronium etc. belong to this category (even Cooper pairs could be said to be in this category since the two electrons making up the pair are distinguishable by spin or momentum). For simplicity, the fermions making up the composite particle are assumed to contain a single degree of freedom such as spin. Both fermions jointly possess other degrees of freedom such as momentum of their center of mass. Internal degrees of freedom encode the internal structure of the composite boson and are as such generally harder to access than the external degrees of freedom.

Numerous experiments on Bose-Einstein condensation of atoms made of an even number of fermions have strengthened the hypothesis that these particles are bosons. However as we have seen, one must be careful when neglecting the internal structure of composite bosons, especially since the properties of a group of composite bosons could be influenced by the Pauli principle acting on the constituent fermions when they are too close to one another. The bosonic behavior of composite bosons such as excitons, especially in the context of Bose-Einstein condensation has been studied (see for example [120]), and it was demonstrated that excitons behave as bosons when their density is low so that the overlap of the fermionic wave functions can be neglected.

In this regard, from a quantum information viewpoint, it is interesting to analyze the states of these composite bosons that lead to "good" bosonic behavior. A careful analysis of the wave functions of experimentally achieved condensates clearly indicates entanglement between certain degrees of freedom of the constituent fermions. This fact was first investigated in [122, 123] where it was hypothesized that the amount of entanglement between the constituent fermions plays a substantial role. It was suggested that a large amount of entanglement is necessary for good bosonic behavior. We first present the mathematical basis for their claim.

A brief introduction to the measure of entanglement that we shall employ is in order. For any pure state of a bipartite quantum system, there exists a useful decomposition known as the Schmidt decomposition which is stated formally as follows (for a proof refer to [32]).

The Schmidt decomposition theorem: Any pure state $|\psi\rangle \in H_1 \otimes H_2$ of a bipartite quantum system can be written in the form

$$|\psi\rangle = \sum_{i=1}^{d} \sqrt{\lambda_i} |i\rangle_1 |i'\rangle_2, \tag{7.1}$$

where $\{|i\rangle_1\}$ and $\{|i'\rangle_2\}$ are sets of orthonormal quantum states in H_1 and H_2 respectively, and λ_i are probabilities (real numbers) satisfying $\lambda_i > 0$ and $\sum_i \lambda_i = 1$.

The λ_i here can also be seen to be the positive eigenvalues of the reduced density matrices of subsystems 1 and 2, which are given by $\rho_1 = \sum_i \lambda_i |i\rangle\langle i|$ and $\rho_2 = \sum_i \lambda_i |i'\rangle\langle i'|$. The number d of such λ_i in the Schmidt decomposition for a state $|\psi\rangle$ is known as its Schmidt number or Schmidt rank [32, 124]. For a pure separable state (a product state), the Schmidt number is 1 while every bipartite pure entangled state has Schmidt number greater than one. The purity of the reduced density matrices ρ_1 and ρ_2 is given by $P = \sum_i \lambda_i^2$ and is a measure of entanglement for bipartite pure states. The smaller the entanglement, the more pure the states of the subsystems and vice versa. This is closely related to a quantity defined in condensed matter physics as the participation ratio, given as $\xi = \frac{1}{\sum_i \lambda_i^2} = \frac{1}{P}$. $\xi = d$ indicates maximal entanglement (the λ_i's then follow the uniform distribution each being equal to $1/d$) and $\xi = 1$ indicates separability. As we are studying pure states, the amount of entanglement can also be quantified by the von Neumann entropy of the reduced density matrix of one of the subsystems, which is given by the Shannon entropy of the probability distribution generated by λ_n, i.e., $S(\rho_1) = -\sum_n \lambda_n \log \lambda_n$. The purity and Schmidt number are used in the following analysis of entanglement in pure states of composite particle systems.

Consider a composite boson (coboson) made of two distinguishable fermions of type A and type B, with associated fermionic creation operators $a^\dagger$ and $b^\dagger$ respectively. The corresponding annihilation operators are the respective Hermitian conjugates. Standard anti-commutation rules apply, i.e., $\{K_n, K_m^\dagger\} = \delta_{nm}$ $(K = a, b)$. Assume that the two fermions are described by a single internal mode encoded in an index n. Then the general pure state of the composite boson is written in Schmidt-decomposed form as

$$|\psi\rangle_{AB} = \sum_n \sqrt{\lambda_n} a_n^\dagger b_n^\dagger |0\rangle, \tag{7.2}$$

where $a_n^\dagger$ ($b_n^\dagger$) creates a particle of type A (B) in mode n and λ_n denotes the probability of occupation of the mode n. The sum in the above equation is over all modes from 0 to ∞, however for ease of calculation, one can introduce a cutoff d (justified on grounds of finite energy), which later can be taken to infinity. The number of non-zero coefficients λ_n is the Schmidt number of this state and so long as it is larger than one, the state is entangled.

A necessary condition for the composite system described by the state $|\psi\rangle_{AB}$ to exhibit good bosonic behaviour is that the creation operator of the composite boson

$$c^\dagger = \sum_n \sqrt{\lambda_n} a_n^\dagger b_n^\dagger$$

mimics an ideal bosonic creation operator as faithfully as possible, i.e., that the commutator $[c, c^\dagger]$ be as close as possible to the identity [121]. The commutation relation is given by $[c, c^\dagger] = \mathbb{1} - \Delta$ where the "bosonic departure" operator $\Delta = \sum_n \lambda_n (a_n^\dagger a_n + b_n^\dagger b_n)$ can be interpreted as the deviation from the ideal bosonic commutation relation and should be as small as possible, in some sense.

An approach to quantifying the smallness of Δ was expounded in [121]. Two operators were considered, the bosonic departure Δ and the boson number $c^\dagger c$, whose expectation value in the cobosonic number states $|N\rangle$ was postulated to be a measure of the quality of bosons.

The composite boson number state is defined as

$$|N\rangle = \chi_N^{-1/2} \frac{c^{\dagger N}}{\sqrt{N!}} |0\rangle.$$

Note that this state resembles a usual bosonic number state except for the normalization factor

$$\chi_N = N! \sum_{n_1 < \cdots < n_N} (\lambda_{n_1} \ldots \lambda_{n_N})$$

where the λ_{n_j} are the Schmidt coefficients of the state $c^\dagger|0\rangle$ from Eqn.(7.2). The behavior of the state $|N\rangle$ under the action of the annihilation operator c is given by

$$c|N\rangle = \alpha_N \sqrt{N} |N-1\rangle + |\varepsilon_N\rangle. \tag{7.3}$$

The parameter $\alpha_N = \sqrt{\frac{\chi_N}{\chi_{N-1}}}$ is a normalization constant and $|\varepsilon_N\rangle$ is a vector orthogonal to $|N-1\rangle$.

$$\langle \varepsilon_N | \varepsilon_N \rangle = 1 - N \frac{\chi_N}{\chi_{N-1}} + (N-1) \frac{\chi_{N+1}}{\chi_N}.$$

The expectation values of the bosonic departure and boson number operators in state $|N\rangle$ are

$$\langle \Delta \rangle_N = 2\left(1 - \frac{\chi_{N+1}}{\chi_N}\right),$$

$$\left\langle c^\dagger c \right\rangle_N = N - \frac{N-1}{2} \langle \Delta \rangle_N .$$

As can be seen from the above equations, the ratio $F_{N+1} = \frac{\chi_{N+1}}{\chi_N}$ is a mathematical indicator of the quality of the boson. In particular, ideal bosonic behavior is obtained when the ratio approaches one. Moreover, $\alpha_N \to 1$ and $\langle \varepsilon_N | \varepsilon_N \rangle \to 0$ as $F_{N+1} \to 1$. The analysis also works for the case of a composite particle made of two distinguishable elementary bosons. In that case, the commutation relation yields $[c, c^\dagger] = \mathbb{1} + \Delta$ with $\Delta = \sum_n \lambda_n (a_n^\dagger a_n + b_n^\dagger b_n)$ as before while here $a^\dagger$ and $b^\dagger$ denote ideal bosonic creation operators obeying $[a, a^\dagger] = \mathbb{1}$ and $[b, b^\dagger] = \mathbb{1}$.

In [122], a particular (exponential) distribution of λ_n was considered, namely $\lambda_n = (1-z)z^n$ with the parameter z defined to be in the range $0 < z < 1$. This parameter determined how quickly λ_n decreased with n. For these states, the Schmidt number was found to be $\kappa = (1+z)/(1-z)$ which is a monotonically increasing function in the range $0 < z < 1$. For $\kappa \gg N$, it was shown that $F_{N+1} \approx 1 - \frac{N}{\kappa}$, from which it was concluded that "the bosonic particle description is valid when the effective number of Schmidt modes is much greater than the total number of composite particles". In other words, it was suggested that the bosonic behavior of composite bosons is related to the entanglement between the constituent fermions and approaches one in the limit of infinite entanglement. Moreover, since in principle entanglement does not depend on the distance between the fermions, it was speculated that highly delocalized composite bosons could be prepared and made to condense. It was also pointed out that the analysis can be extended to the scenario of composite bosons made of two distinguishable bosons where again ideal bosonic behavior is recovered in the limit of large entanglement.

This speculation relating entanglement and bosonic behavior was confirmed by a more general investigation into all possible distributions of λ_n in [123]. It was shown that the ratio $F_{N+1} = \chi_{N+1}/\chi_N$ can in general be bounded from above and below by simple functions of the purity $P(\rho) = \mathrm{Tr}\{\rho^2_{A(B)}\} = 1/\kappa$ of the reduced density matrix $\rho_{A(B)}$ of particle A (B), the entanglement measure for pure bipartite states. The result was

$$1 - NP \leq F_{N+1} \leq 1 - P. \tag{7.4}$$

For highly entangled states, i.e., for which $P \to 0$, the inequalities imply that $F_{N+1} \to 1$. In fact, as shown in [118] one can obtain better approximations to the ratio F_{N+1} for large N by making use of the Newton-Girard identity [125] that relates the elementary symmetric polynomials χ_N to the complete symmetric polynomials $P_j = \sum_{m=0}^{\infty} \lambda_m^j$ (note that P_2 is the purity P). This identity can be written as

$$\frac{\chi_{N+1}}{(N)!} = \sum_{j=1}^{N+1} (-1)^{j-1} P_j \frac{\chi_{N+1-j}}{(N+1-j)!}.$$

Dividing the above equation throughout by χ_{N+1} and noting that for large N, $\frac{\chi_{N+1}}{\chi_{N+1-j}} \approx \left(\frac{\chi_{N+1}}{\chi_N}\right)^j$, we obtain

$$\frac{1}{F_{N+1}} - \frac{NP_2}{F^2_{N+1}} + \frac{N^2P_3}{F^3_{N+1}} - \frac{N^3P_4}{F^4_{N+1}} + \cdots \approx 1.$$

As we shall see in the following sections, a necessary condition for good bosonic behaviour is that for all n, $\lambda_n \ll 1/N$, which implies that the terms $N^{j-1}P_j$ in the expression above decrease in magnitude sharply [126]. For instance, for a typical λ_k of the order $O(1/N^2)$, the expression $N^{j-1}P_j$ is of the order of $O(1/N^{j-1})$. Hence, performing a series expansion around these small terms leads to

$$F_{N+1} \approx 1 - NP_2 + N^2(P_3 - P_2^2) + O(N^3\,(P_4 + 2\,P_2^3 - 3\,P_2\,P_3)),$$

from which the inequalities (7.4) can be recovered. Better approximations to this important ratio for large N (which is typically the case one is interested in) can be made by considering more terms in the series expansion above. The bounds in (7.4) seem to validate the hypothesis that the bosonic behavior depends on the entanglement between

A and B. However, a more thorough investigation of the set of states required for good bosonic behavior is required and we shall proceed to do this. We shall find that entanglement is only part of the picture, i.e., while large entanglement between the constituent fermions is necessary for good bosonic behavior, it is not sufficient [118].

Before we proceed to that however, let us note an interesting aside, namely that composite particles made of three distinguishable fermions always behave like a fermion, irrespective of the (pure) state they are in. To see this, let us write the general pure state of such a composite particle as

$$d^\dagger = \sum_{p,q,r} \lambda_{pqr} a_p^\dagger b_q^\dagger c_r^\dagger,$$

where λ_{pqr} are complex amplitudes satisfying the normalization constraint $\sum_{p,q,r} |\lambda_{pqr}|^2 = 1$. We can now calculate the anti-commutator $\{d, d^\dagger\}$ as

$$\begin{aligned}\{d, d^\dagger\} = \mathbb{1} \quad &- \sum_{p,q,r,p',q',r'} \lambda^*_{p'q'r'} \lambda_{pqr} (\delta_{pp'} \delta q q' c_r^\dagger c_{r'} + \delta_{qq'} \delta_{rr'} a_p^\dagger a_{p'} + \delta_{pp'} \delta_{rr'} b_q^\dagger b_{q'}) \\ &+ \sum_{p,q,r,p',q',r'} \lambda^*_{p'q'r'} \lambda_{pqr} (\delta_{pp'} b_q^\dagger c_r^\dagger c_{r'} b_{q'} + \delta_{qq'} a_p^\dagger c_r^\dagger c_{r'} a_{p'} + \delta_{rr'} a_p^\dagger b_q^\dagger b_{q'} a_{p'}).\end{aligned}$$

It is now easy to check that $(d^\dagger)^2 = 0$ meaning that one cannot create a state consisting of more than one composite particle of this type. Moreover, the average value of the anti-commutator in state $|1\rangle$ is also unity implying that particles of this type always behave like fermions. It is an interesting open question to check if it is always the case that composite particles of an arbitrary odd number of fermions (distinguishable or indistinguishable) behave like fermions.

We now return to our consideration of the system of composite bosons made of two distinguishable fermions and try to identify the states that result in ideal bosonic behavior of these particles. Unlike in the previous approach which focused on mathematical aspects such as the commutation relation, we concentrate on the physical aspect of the display of bosonic properties, such as the formation of a condensate. This new approach clarifies the importance of entanglement and allows us to link it to other criteria discussed in the literature. As we shall see, the phenomenon of monogamy of entanglement plays a crucial role in the display of bosonic behavior. Despite the fact that one cannot access the internal structure of the composite bosons and therefore cannot directly influence the entanglement between fermions, this inevitably happens when two or more composite bosons are forced to occupy the same external state. This phenomenon is related to two fundamental properties of quantum particles, namely indistinguishability and monogamy of entanglement.

Fig.(7.1) depicts this situation. In Fig.(7.1)(a), two cobosons (each made of two distinguishable fermions denoted by circles and stars) occupy different external states so that

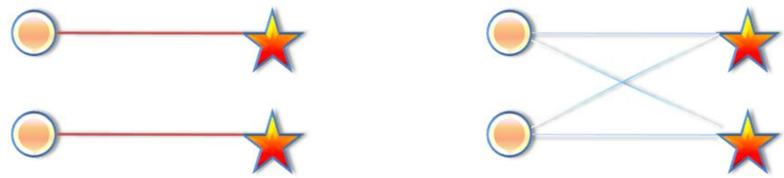

Figure 7.1: An illustration of how indistinguishability and monogamy affect the entanglement in a pair of composite bosons. In (a) the solid red connecting line between fermions of type A (circles) and those of type B (stars) indicates strong entanglement within the coboson. In (b) the dashed blue line between fermions indicates that the indistinguishability and monogamy of entanglment force the redistribution of entanglement so that the entanglement within a pair is no longer large.

there exists a parameter which in principle allows one to distinguish between two fermions of the same type. The solid red connecting line denotes initial strong entanglement within each coboson. In Fig.7.1(b), both cobosons occupy the same external state. Indistinguishability and monogamy of entanglement force the entanglement to be redistributed over all possible pairs of distinguishable fermions. This is illustrated by the dashed blue lines which denote weaker entanglement. This same phenomenon occurs when an arbitrary large number of cobosons is considered such as in a condensate. It is therefore intuitively clear that to preserve large entanglement within each particle, the composite bosons must not be packed with high density. In principle, fermions of different type do not have to interact (although fermions of the same type can interact via Pauli exchange) in the process in which the corresponding composite bosons occupy the same state. Therefore, it is valid to consider the process of bunching and condensation in the quantum information theoretic framework of local quantum operations and classical communication (LOCC).

7.2 Condensation by LOCC.

Let us introduce condensation as a generalization of the situation considered in Fig. 7.1. We refer to the process of generating the state $|N\rangle$ from N single-particle composite boson states $|\psi\rangle_{AB}^{\otimes N}$ as the process of creating a condensate. This is a simplified notion of the actual picture, since we do not consider parameters such as temperature, however this simplification captures one of the characteristic features of the condensation process with regard to the macroscopic occupation of a single state. Consider a scenario in which there is no interaction between fermions of type A and B since condensation should be possible even in the absence of such interaction (Fig. 7.2). This would imply local operations among fermions of type A and B only. This formalism nicely incorporates the unavoidable Pauli interactions among fermions of a specific type. A notable characteristic of the LOCC operations is that entanglement in the partition $A-B$ cannot be increased because this

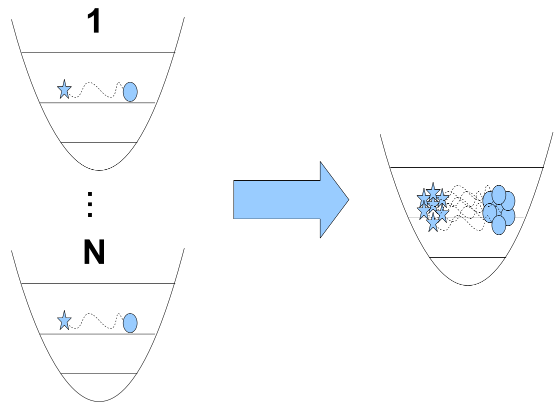

Figure 7.2: A simplified picture of the condensation process in composite bosons. N composite bosons in N different wells are brought via an LOCC process into a single well. In this process, no interactions between fermions of different type is assumed although fermions of the same type can interact via Pauli exchange.

would require interaction between these subsystems.

The necessary and sufficient criterion for the existence of a deterministic LOCC transformation between bipartite quantum states was given in [127] in terms of the mathematical technique of majorization. For the composite bosons to behave like real bosons, the deterministic LOCC process of formation of N-particle composite boson states $|N\rangle$ must be possible, i.e., it should be possible to condense the composite bosons in the absence of interactions between subsystems A and B. Therefore, the corresponding final and initial composite boson states would have to obey the majorization criterion.

Let us start with N identical composite bosons in N different potential wells. This situation is illustrated in Fig.(7.2) which is a schematic picture presenting the idea of condensation of composite bosons. Each composite boson initially occupies a different potential well. The well energy levels enumerated by n give rise to the internal structure of composite bosons $c^\dagger = \sum_n \sqrt{\lambda_n} a_n^\dagger b_n^\dagger$. We will investigate the possibility of an LOCC operation bringing all composite bosons into one well as in the right of the figure.

The initial state is $c_1^\dagger c_2^\dagger \ldots c_N^\dagger |0\rangle$ where $c_j^\dagger = \sum_n \sqrt{\lambda_n} a_n^{(j)\dagger} b_n^{(j)\dagger}$ creates one composite particle in the j^{th} well. Our goal is to condense all composite bosons into a single well by an LOCC process, i.e., to obtain the final state $(c^\dagger)^N|0\rangle$ (up to normalization). The majorization criterion states that a bipartite state $|\psi\rangle_{AB}$ can be transformed by LOCC into another bipartite state $|\phi\rangle_{AB}$ if and only if the vector of eigenvalues of the density matrix of one of the two subsystems of state $|\psi\rangle_{AB}$, denoted by $\vec{\lambda}_\psi$, is majorized by the corresponding vector $\vec{\lambda}_\phi$ of state $|\phi\rangle_{AB}$. This mathematical condition is written as $\vec{\lambda}_\psi \prec \vec{\lambda}_\phi$, meaning that for all $k = 0, 1, 2, \ldots, d-2$, $\sum_{j=0}^{k} \lambda_j^\downarrow(\psi) \leq \sum_{j=0}^{k} \lambda_j^\downarrow(\phi)$, with equality when $k = d-1$, $\sum_{j=0}^{d-1} \lambda_j^\downarrow(\psi) = \sum_{j=0}^{d-1} \lambda_j^\downarrow(\phi) = 1$. Here the symbol $\downarrow$ indicates that the eigenvalues are enumerated in decreasing order, i.e., $\lambda_0 \geq \lambda_1 \geq \cdots \geq \lambda_{d-1}$. One can verify that majorization applies to fermionic systems. This can be seen by noting that the necessary transformations [127] can first be performed while the composite particles occupy different wells when there exists a parameter which allows to distinguish between different composite bosons. Thereafter, it is possible to perform a one-to-one mapping from N wells into one.

The initial and final reduced density matrices of subsystem A or B (ρ_i and ρ_f) in the process of condensation considered here are given by the diagonal matrices

$$\rho_i = \sum_{n_1,n_2,\dots,n_N} \lambda_{n_1}\lambda_{n_2}\dots\lambda_{n_N} a^{(1)\dagger}_{n_1} a^{(2)\dagger}_{n_2}\dots a^{(N)\dagger}_{n_N}|0\rangle\langle 0| a^{(N)}_{n_N}\dots a^{(2)}_{n_2} a^{(1)}_{n_1},$$

and

$$\rho_f = \frac{1}{\tilde{\chi}_N} \sum_{n_1<n_2<\dots<n_N} \lambda_{n_1}\lambda_{n_2}\dots\lambda_{n_N} a^{\dagger}_{n_1} a^{\dagger}_{n_2}\dots a^{\dagger}_{n_N}|0\rangle\langle 0| a_{n_N}\dots a_{n_2} a_{n_1},$$

where $\tilde{\chi}_N = \sum_{n_1<\dots<n_N} \lambda_{n_1}\dots\lambda_{n_N}$ is a normalization factor related to χ_N via $\chi_N = N!\tilde{\chi}_N$. In the second equation above, the superscript on the operators is omitted, since all operators correspond to composite bosons in one well. In this sense, condensation can be thought of as a process in which the composite bosons lose their identity and become indistinguishable once all of them are in the same well. With the λ's being enumerated in descending order, the ordered vectors of eigenvalues for the initial ($\vec{\lambda}_i$) and final ($\vec{\lambda}_f$) states are given by $\vec{\lambda}_i = \{\lambda_0^N, \lambda_0^{N-1}\lambda_1, \dots\}$, and $\vec{\lambda}_f = \frac{1}{\tilde{\chi}_N}\{\lambda_0\lambda_1\dots\lambda_{N-1}, \dots\}$. Note that here the vector $\vec{\lambda}_i$ is d^N-dimensional and $\vec{\lambda}_f$ is $\begin{pmatrix} d \\ N \end{pmatrix}$-dimensional. The dimension of the second vector being smaller than that of the first, we augment $\vec{\lambda}_f$ by $d^N - \begin{pmatrix} d \\ N \end{pmatrix}$ zeros as required for comparing the two vectors by the majorization criterion. In the following, we shall look for composite boson states described by distributions $\{\lambda\}$ for which $\vec{\lambda}_i \prec \vec{\lambda}_f$.

Entanglement and majorization. We first provide an explicit counterexample showing that small purity P does not imply majorization, i.e., we find composite boson states for which the purity is small but vectors $\vec{\lambda}_i$ and $\vec{\lambda}_f$ corresponding to $|\psi\rangle_{AB}^{\otimes N}$ and $|N\rangle$, respectively, do not obey the majorization criterion. These states are described by the distribution $\{\lambda\}$ given as

$$\lambda_j = \frac{1}{(j+1)^s\zeta(s)}, \tag{7.5}$$

where $\zeta(s) = \sum_{j=0}^{\infty}\frac{1}{(j+1)^s}$ is the Riemann Zeta function (giving rise to the Zipf distribution). For $s>1$ the λ_j-series sums to one and is a valid probability distribution. The purity for these states $P_s = \zeta(2s)/\zeta(s)^2$ can be made small by choosing $s = 1+\varepsilon$ ($0<\varepsilon\ll 1$), since $P_{1+\varepsilon} \approx \zeta(2)\varepsilon^2 = \frac{\pi^2}{6}\varepsilon^2$.

For simplicity, we consider the violation of the majorization relation between the first elements of the vectors, i.e.,

$$\lambda_0^N > \frac{\lambda_0\dots\lambda_{N-1}}{\tilde{\chi}_N}. \tag{7.6}$$

Noting that λ_j's are arranged in descending order, we can write $\lambda_j := \lambda_0\gamma_j$, with $0 \leq \gamma_j \leq 1$, $\gamma_{j+1} \leq \gamma_j$ and $\gamma_0 = 1$. Therefore, the above formula for the violation of the majorization criterion can be rewritten as $\tilde{\chi}_N > \gamma_1\gamma_2 \ldots \gamma_{N-1}$. Using (7.4), one finds that $\tilde{\chi}_N \geq \tilde{\chi}_{N-1}\left(\frac{1+P}{N} - P\right)$. Applying this relation N times gives $\tilde{\chi}_N \geq \frac{P^{N-1}}{N!} \frac{\Gamma(1/P)}{\Gamma(1/P-(N-1))}$ where $\Gamma(x)$ denotes the Gamma function. Hence, we see that majorization fails if

$$\gamma_1\gamma_2 \ldots \gamma_{N-1} < \frac{1}{N!}\left(1-(N-1)P\right)^{N-1}. \tag{7.7}$$

Plugging $P_{1+\varepsilon}$ into (7.7) gives $N!^{\varepsilon}[1-(N-1)P_{1+\varepsilon}]^{N-1} > 1$. For $N\varepsilon \leq 1$, we expand the above into power series and keep only the terms up to first order to obtain $1+\varepsilon\log(N!) > 1$. It is clear that the majorization condition is violated. Note also that from the lower bound in (7.4), we have

$$F_{N+1} \geq 1 - \frac{\pi^2}{6}(N+1)\varepsilon^2.$$

For $(N+1)\varepsilon^2 \ll 1$, the important ratio F_{N+1} can be made arbitrarily close to one even though majorization is not possible. In this sense, the majorization provides an additional and independent criterion from the one discussed previously, which was in terms of the ratio F_{N+1}.

Density of composite bosons and entanglement. It has been argued [128, 129] that a necessary condition for bosonic behavior of composite bosons (in particular, of excitons) is that for all k,

$$N\lambda_k \ll 1. \tag{7.8}$$

This condition is related to the physical requirement that the density of composite bosons be low in order to prevent overlap between wavefunctions of the constituent fermions.

We now show that this condition is more general than large entanglement, in that it implies $NP \ll 1$, while the converse is not necessarily true. This can be seen by showing that the purity is bounded from above by the largest coefficient λ_0. Since $\sum_j \lambda_j = 1$, we have $\sum_j \gamma_j = \frac{1}{\lambda_0}$ and the following holds

$$P = \sum_j \lambda_j^2 = \lambda_0^2 \sum_j \gamma_j^2 \leq \lambda_0^2 \sum_j \gamma_j = \lambda_0.$$

Therefore $P \ll \frac{1}{N}$ is guaranteed if $\lambda_0 \ll \frac{1}{N}$.

However, the converse is not true ($NP \ll 1$ does not imply $N\lambda_0 \ll 1$). To see this, let us consider the states in Eqn.(7.5) for $s = 1+\varepsilon$. For $\varepsilon = \frac{1}{N}$ the purity is $O(1/N^2)$, but the condition $N\lambda_k \ll 1$ is not satisfied, because $\lambda_0 = \frac{1}{\zeta(1+\varepsilon)} \approx \varepsilon$ and $N\lambda_0 \approx 1$.

Physical criterion for majorization. In this section, we would like to give a sufficient condition for majorization that has a simple physical interpretation in terms of the density of composite bosons. To do so, let us begin by considering the situation when d and N are finite, and then take the limit $d \to \infty$ and $N \to \infty$ while keeping the ratio $\mu = \frac{N}{d}$

constant. μ is a quantity proportional to the density of composite bosons $\rho = N/V$ since $\mu = \frac{\rho}{\omega}$, where ω is the density of states.

We begin with the state described by the vector $\vec{\lambda} = \{\lambda_0, \ldots, \lambda_d\}$. Firstly, note that if it were possible, by LOCC, to transform $\vec{\lambda}_i$ to a vector $\vec{u}_f = \left\{ \binom{d}{N}^{-1}, \ldots, \binom{d}{N}^{-1} \right\}$, it would also be possible to transform via LOCC $\vec{\lambda}_i$ to $\vec{\lambda}_f$ via LOCC processes. This is because the vector $\vec{u}_f$ corresponds to the uniform distribution in the final Hilbert space and is therefore guaranteed to be majorized by $\vec{\lambda}_f$. Note that the distribution $\vec{u}_f$ corresponds to the state with the highest F_N and is expected to be the most ideal composite boson condensate. The majorization problem $\vec{\lambda}_i \prec \vec{u}_f$ yields a simple condition $\lambda_0^N \leq \binom{d}{N}^{-1}$ which in the infinite limit translates simply to

$$\begin{aligned} \lambda_0 \leq \mu \left(1-\mu\right)^{\frac{1-\mu}{\mu}} \ \ (< \mu) \\ \lambda_0 \leq \mu. \end{aligned} \tag{7.9}$$

This condition states that majorization is guaranteed when the probability of occupation of the ground state is less than the density μ. It supports the idea of a critical density for condensation, that is, $\lambda_0 \leq \mu$ may be satisfied for all densities above a critical value μ_{cr}, ensuring that such distributions lead to condensation without interaction between the fermions as required for proper bosonic behavior.

Classes of states that obey majorization. There exist certain classes of states that always obey the majorization condition. Let us consider the states introduced in [122], defined by $\lambda_j = (1-z)z^j$ $(0 < z < 1)$. For these, $\tilde{\chi}_N = \frac{z^{N(N-1)/2}(1-z)^N}{\prod_{j=1}^{N}(1-z^j)}$, and the purity is given by $P_z = \frac{1-z}{1+z}$. These states obey the majorization criterion for all z and N. To see this, let us firstly observe that $\vec{\lambda}_i = (1-z)^N\{1, z, z, \ldots, z, z^2, z^2, \ldots\}$, where the degeneracy of z^l is $g_l^{(i)} = \binom{l+N-1}{l}$. On the other hand, $\vec{\lambda}_f = \frac{(1-z)^N z^{N(N-1)/2}}{\tilde{\chi}_N}\{1, z, z^2, z^2, \ldots\}$, for which the degeneracy of z^l $(g_l^{(f)})$ is smaller than $g_l^{(i)}$. Majorization states that, for all k, the sum of the first k terms of $\vec{\lambda}_i$ has to be less than, or equal to the sum of the first k terms of $\vec{\lambda}_f$. Canceling common factors, the overall multiplicative factor in $\vec{\lambda}_f$ is $\frac{z^{N(N-1)/2}}{\tilde{\chi}_N} = \prod_{k=1}^{N-1}\sum_{j=0}^{k} z^j$, and we can rewrite $\vec{\lambda}'_i = \{1, z, z, \ldots, z, z^2, z^2, \ldots\}$, and $\vec{\lambda}'_f = \left(\prod_{k=1}^{N-1}\sum_{j=0}^{k} z^j\right)\{1, z, z^2, z^2, \ldots\}$. Next, notice that the sum over all terms of both vectors is the same and equal to $1/(1-z)^N$. Moreover, this sum can be written as a unique polynomial $\frac{1}{(1-z)^N} = \sum_{j=0}^{\infty} g_j^{(i)} z^j$. The sum of first k terms of $\vec{\lambda}'_i$ is given by $\sum_{j=1}^{k}[\vec{\lambda}'_i]_j = \sum_{j=0}^{l-1} g_j^{(i)} z^j + (k - \sum_{j=0}^{l-1} g_j^{(i)}) z^l$. Due to the multiplicative factor of $\vec{\lambda}'_f$ and the fact that the degeneracy of $\vec{\lambda}'_f$ is less than that of $\vec{\lambda}'_i$, we have $\sum_{j=1}^{k}[\vec{\lambda}'_i]_j < \sum_{j=1}^{k}[\vec{\lambda}'_f]_j$ which ends the proof. We have thus shown that exponential distributions obey the majorization relation for any z and N. Therefore, the set of states that obey both criteria, i.e., the one in terms of F_{N+1} and the one related to majorization, is non-empty and captures the set of physical states that are good composite bosons.

A sufficient criterion for majorization. Let us finally note a sufficient condition for majorization. If there exists an i ($1 \leq i \leq n$) such that for all $k \leq i$, $\sum_{j=1}^{k} x_j \leq \sum_{j=1}^{k} y_j$, and for $k > i$, $\sum_{j=i+1}^{n} x_j \geq \sum_{j=i+1}^{n} y_j$, then $\vec{x} \prec \vec{y}$ [130]. This implies that any distribution of $\lambda' s$ with $\lambda_0 \leq (1-z)$ (with $z \to 1$) and with only one intersection with the exponential distribution will be majorized by the latter. This suggests the interesting possibility that certain states, while not obeying majorization themselves, could be transformed by LOCC into states that do, and can therefore be considered as good cobosonic states capable of forming a condensate, i.e., $c \to c' \to c'^N$. This phenomenon of "distilling" good bosons by distilling the entanglement between the fermions by LOCC operations, merits further investigation.

7.3 Addition and subtraction of composite particles

Let us now proceed to the study of bosonic and fermionic behavior for more general composite particle systems following the analysis in [119]. An interesting way to quantify the bosonic and fermionic behavior of a composite particle is via the operations of single particle addition and subtraction. For fermions, the addition of a single particle to a mode that is already occupied is forbidden by the Pauli exclusion principle while for bosons, it is easier to add a particle to an already occupied state than it is for distinguishable classical particles. This fact can be used to formulate a measure of bosonic and fermionic quality based on single particle addition followed by subtraction. This measure reveals that the composite particles can exhibit a variety of behaviors ranging from fermionic to bosonic depending on the physical situation and the state of the system at hand.

The operations of single particle addition and subtraction are known to be probabilistic and are best described by the language of completely positive maps and Kraus operators. The success probability of these operations is related to the quality of fermionic or bosonic behavior of the particles. In this section, we construct optimal bosonic quantum channels to implement these operations and apply them to formulate a measure of bosonic and fermionic quality. For composite particles made of two distinguishable fermions or two distinguishable bosons the value of the measure depends on the entanglement between the constituents. We identify a critical amount of entanglement for which the transition from fermionic to bosonic behavior occurs for composite particles of two distinguishable fermions.

Addition and subtraction channels:

In general, the processes of particle addition and subtraction are not deterministic. Moreover, they cannot be formulated simply as Kraus operators K_j which describe non-deterministic evolutions in terms of completely positive quantum channels $\rho' = \sum_j K_j \rho K_j^\dagger$

[32]. The reason is that Kraus operators $\{K_0, K_1, \dots\}$ which describe a quantum channel cannot increase the norm of the state, i.e., $\sum_j K_j^\dagger K_j \leq I$. Setting $K_0 = a^\dagger$ yields $K_0^\dagger K_0 = aa^\dagger = N + 1$, where $a^\dagger$ denotes the creation operator for a single ideal boson. The eigenvalues of the bosonic particle number operator N lie in the set of all nonnegative integers, which together with the requirement that the norm cannot increase immediately implies the negativity of the remaining operators $K_j^\dagger K_j$ for $j \neq 0$. The case of the annihilation process is analogous. It is interesting that the probabilistic nature of the operators $a^\dagger$ and a can also be deduced from the fact that deterministic addition and subtraction could lead to an increase of entanglement via local operations. This can be seen for example by considering the state of a single particle in two modes A and B, $|\psi\rangle = \alpha|0_A 1_B\rangle + \beta|1_A 0_B\rangle$ with real positive parameters α and β satisfying $\alpha^2 + \beta^2 = 1$ and $\alpha^2 > 4\beta^2$. This state has entanglement measured by the concurrence [28] given as $2\alpha\beta$. It is clear that a local operation of addition followed by subtraction at mode A leads to the state $|\psi_{AS}\rangle = \frac{1}{\sqrt{\alpha^2+4\beta^2}}(\alpha|0_A 1_B\rangle + 2\beta|1_A 0_B\rangle)$ with entanglement measured by concurrence given as $\frac{4\alpha\beta}{\alpha^2+4\beta^2}$ which is larger than the initial entanglement. Therefore, the probabilistic nature of the operators $a^\dagger$ and a is needed to ensure that entanglement does not increase via local operations.

Any operator which effectively adds one particle to the system can be written as

$$a_{eff}^\dagger = \sum_{n=0}^{\infty} f_n |n+1\rangle\langle n|. \tag{7.10}$$

An effective annihilation operator is the hermitian conjugate of the above. This operator is a valid Kraus operator (satisfying $\sum_j K_j^\dagger K_j \leq I$) if $|f_n|^2 \leq 1$ for all n. Note that operationally $\frac{|f_n|^2}{|f_{n-1}|^2}$ corresponds to the ratio of probabilities $\frac{p_{n\to n+1}}{p_{n-1\to n}}$, where $p_{n\to n+1}$ denotes the probability of adding a single particle to a mode in which there are already n particles. It is convenient to rewrite (7.10) in the following form

$$a_{eff}^\dagger = g(N)a^\dagger = \sum_{n=0}^{\infty} g(n+1)\sqrt{n+1}|n+1\rangle\langle n|,$$

where $g(N)$ is a function of the particle number operator. The extreme case of an operator in which all multiplicative factors are equal to one corresponds to the creation operator of distinguishable particles $a_d^\dagger$, where $g(N) = 1/\sqrt{N}$.

To implement a perfect bosonic channel we would like to have the ratios to be $\frac{f_n}{f_{n-1}} = \frac{\sqrt{n+1}}{\sqrt{n}}$. In this case $g(N)$ is a constant, however the normalization constraint and the fact that the sum over n goes to infinity imply that the only possible solution is $g(N) = 0$. This problem can be circumvented if the maximal number of particles is bounded. In this case, the optimal operator $a_{eff}^\dagger$ is state dependent, i.e., for the state supported on the subspace spanned by $\{|0\rangle, |1\rangle, \dots, |n_{max}\rangle\}$ the corresponding function is $g(N) = \frac{1}{\sqrt{n_{max}+1}}$, a constant for $n \leq n_{max}$, and $g(N) = \frac{1}{\sqrt{N}}$ for $n > n_{max}$. The effective operator $a_{eff}^\dagger$ with this function is then the optimal operator to implement particle addition and its conjugate is the optimal particle subtraction operator. Finally, note that in case of fermions the maximal number of particles in a single mode is naturally bounded by 1, therefore fermionic creation and annihilation operators are already optimal Kraus channels. We now proceed to formulate a measure of bosonic and fermionic quality of particles based on these optimal addition and subtraction quantum channels.

Let us quantify the behavior of particles under the operations of one-particle addition and subtraction to a single mode. We compare the resulting state after particle addition followed by subtraction (AS) with the initial state of the particles which we assume to be in a mixed state $\rho = \sum_n p_n |n\rangle\langle n|$. The reason for this assumption is that in general the particles under consideration can be massive and superselection rules prevent us from preparing superpositions of different particle-number states. Note that this measure is operationally similar to the commutator approach except that we ignore the operation of subtraction followed by addition (SA). Note that the operation AS for distinguishable particles, described by the creation operator $c_d^\dagger = \sum_{n=0}^{\infty} |n+1\rangle\langle n|$ and the corresponding annihilation operator, leaves the initial state unchanged unlike in the case of ideal bosons. However, the action of SA changes even the state of distinguishable particles. A successful subtraction indicates the absence of vacuum in the initial state and one has to update and re-normalize the state of the system. This lower bound on the number of particles is the heart of the classical lack of commutation of particle addition and subtraction $[a_d, a_d^\dagger] = |0\rangle\langle 0|$. In order to get rid of this classical component in a test of bosonic commutation relations, one has to consider states that do not contain any vacuum. We therefore get rid of this subtlety by only considering the operations of addition followed by subtraction.

To detect the change caused by AS it is sufficient to measure the probability distribution of the number of particles $\{p_0, p_1, \dots\}$, where p_n denotes the probability of detecting n particles. In order to develop a measure that is independent of whether the particles are bosons or fermions, we restrict our considerations to p_0 and p_1 alone. Interestingly, although the number of particles involved in the measure is small, for composite particles made of two fermions such as hydrogen atoms, positronium atoms and excitons, we find that the measure provides us with information about the behavior of many-particle Fock states of these composite particles as well.

We begin by defining the following quantity

$$M = p_0 - p_0^{AS},$$

where p_0^{AS} denotes the vacuum occupancy after AS. The value of M is zero for distinguishable particles (with associated creation operators $c_d^\dagger = \sum_n |n+1\rangle\langle n|$). This is because these operators do not alter the probability distribution in the state upon addition and subtraction. We now argue that M is a measure of bosonic and fermionic quality in this scenario. For bosons the action of AS affects the probability distribution in the following manner: $p_n \to (n+1)^2 p_n$, which together with normalization implies a decrease in p_0. Due to the normalization the change in p_0 depends on the total probability distribution $\{p_n\}$. Note that

$$M = p_0 - \frac{p_0}{\sum_{k=0}^{n_{max}} (k+1)^2 p_k} = p_0 - \frac{p_0}{\langle (N+1)^2 \rangle},$$

where N denotes the particle number operator and n_{max} denotes the maximum number of particles in the system. M is maximized for $p_0 = \frac{n_{max}+1}{n_{max}+2}$ and $p_{n_{max}} = 1 - p_0$. The greater the n_{max}, the greater the change in p_0 after AS. Since we restrict ourselves to p_0 and p_1 only, the optimal probability distribution is $\{p_0 = \frac{2}{3}, p_1 = \frac{1}{3}\}$, for which $M = \frac{1}{3}$ in case of perfect bosons. We therefore fix $p_0 = \frac{2}{3}$, and calculate *the measure with respect to the state*

$$\rho_{\mathcal{M}} = \frac{2}{3}|0\rangle\langle 0| + \frac{1}{3}|1\rangle\langle 1|. \tag{7.11}$$

For convenience, we now redefine the measure as $\mathcal{M} = 3M$

$$\mathcal{M} = 2 - 3p_0^{AS}, \tag{7.12}$$

so that for ideal bosons $\mathcal{M} = 1$. For ideal fermions, successful addition to a state of the form (7.11) implies that there is no vacuum in the resulting state. Since at most one fermion can occupy a particular state, the only possible state is $|1\rangle$. It follows that subsequent particle subtraction leads to $p_0^{AS} = 1$ and to $\mathcal{M} = -1$.

Thus far, we have seen that the three values of $\mathcal{M}$, namely 1, 0 and -1 correspond to bosons, distinguishable particles and fermions, respectively. However, the measure is not bounded to these values and in general depends on the probability of AS. Our considerations are restricted to the two probabilities of addition $p_{0\to1}$ and $p_{1\to2}$, and the two probabilities of subtraction $p_{2\to1}$ and $p_{1\to0}$. Since $p_{i\to j} = p_{j\to i}$ we are left with two free parameters $p_{0\to1}$ and $p_{1\to2}$. For the state (7.11)

$$p_0^{AS} = \frac{\frac{2}{3}p_{0\to1}^2}{\frac{2}{3}p_{0\to1}^2 + \frac{1}{3}p_{1\to2}^2} = \frac{2}{2+\mathcal{R}^2},$$

where

$$\mathcal{R} = \frac{p_{1\to2}}{p_{0\to1}} = \frac{|\langle 2|a^\dagger|1\rangle|^2}{|\langle 1|a^\dagger|0\rangle|^2}, \quad 0 \leq \mathcal{R}. \tag{7.13}$$

Therefore, the measure $\mathcal{M}$ reads

$$\mathcal{M} = \frac{2(\mathcal{R}^2 - 1)}{2 + \mathcal{R}^2}, \quad -1 \leq \mathcal{M} < 2. \tag{7.14}$$

We now discuss the various domains of validity of $\mathcal{M}$. Note that $\mathcal{M} < 0$ if $\mathcal{R} < 1$, which happens when $p_{1\to2} < p_{0\to1}$. Intuitively, in this regime it is harder to add a single particle to the mode when there is already one particle in it, which is an indication of fermionic behavior. The critical case when it is impossible to add a particle when there is already one other particle in the mode ($p_{1\to2} = 0$) corresponds to true fermions. On the other hand, $\mathcal{M} > 0$ if $\mathcal{R} > 1$, which happens if $p_{1\to2} > p_{0\to1}$. This corresponds to the situation in which it is easier to add a single particle to the mode when there is already one particle in it, an indication of bosonic behavior. Therefore, we can define domains $\mathcal{M} \in (-1, 0)$ and $\mathcal{M} \in (0, 1)$ as regions of *sub-fermionic* behavior and *sub-bosonic* behavior, respectively. Interestingly, if $\mathcal{R} > 2$ then $\mathcal{M} \in (1, 2)$. In this regime, it becomes easier to add a particle than in the case of true bosons, i.e., the probability of addition when there is already one particle in the system is larger than for ideal bosons; we might call this the *super-bosonic* regime. In the following sections we examine systems which can exhibit sub-fermionic, sub-bosonic and super-bosonic behaviors.

Composite particles of two distinguishable fermions. Let us now examine situations for which $\mathcal{M} \in (-1, 1)$, i.e., the system of composite particles made of two distinguishable fermions in the state

$$|\psi\rangle_{AB} = \sum_k \sqrt{\lambda_k} a_k^\dagger b_k^\dagger |0\rangle. \tag{7.15}$$

The modes k can refer for instance to energy levels of a confining potential, or to the position of the center of mass of A and B. The operation of addition of these composite particles is described by the Kraus channel

$$K_0 = c_{eff}^\dagger = \sum_{n=0}^{n_{max}} g(n+1)\alpha_{n+1}\sqrt{n+1}|n+1\rangle\langle n|,$$

where the state of n composite bosons is given as before by $|n\rangle = \chi_n^{-1/2} \frac{c^{\dagger n}}{\sqrt{n!}}|0\rangle$. The terms $|\varepsilon_n\rangle$ that appear in the action of the annihilation operator on $|n\rangle$ in Eqn. (7.3) can be incorporated into other Kraus operators. The particle subtraction channel is given by taking hermitian conjugate of the above. The optimal function corresponding to realistic implementation of the addition operator, is a constant $g(n+1) = g$.

We are interested in the states $|0\rangle$, $|1\rangle$ and $|2\rangle$, and in parameter χ_2. Note that $\chi_1 = 1$, $c^\dagger|0\rangle = |1\rangle$ and $c|1\rangle = |0\rangle$ follow from the definitions of the creation operator and the number states. Moreover, we do not consider vectors $|\varepsilon_n\rangle$ which are interpreted as states resulting from an unsuccessful subtraction. Effectively, we describe successful addition to the one-particle state and successful subtraction from the two-particle state as

$$c^\dagger|1\rangle = \sqrt{2\chi_2}|2\rangle, \qquad c|2\rangle = \sqrt{2\chi_2}|1\rangle. \tag{7.16}$$

The optimal Kraus channel for addition of these composite particles is then given by

$$K_0 = c_{eff}^\dagger = g|1\rangle\langle 0| + g\sqrt{2\chi_2}|2\rangle\langle 1|. \tag{7.17}$$

The parameter χ_2 is related to the entanglement between the two constituent fermions as

$$\chi_2 = 2\sum_{k>l}\lambda_k\lambda_l = \sum_{k,l}\lambda_k\lambda_l - \sum_k \lambda_k^2 = 1 - P, \tag{7.18}$$

where $0 < P \leq 1$ denotes purity. For $P = 1$ there is no entanglement between A and B, whereas for $P \to 0$ the entanglement between A and B goes to infinity (for the singlet state of two qubits $P = \frac{1}{2}$). Hence P and in consequence χ_2 measure the amount of entanglement between the constituent fermions.

Although we consider only the case of vacuum, single particle and two particles, the value of $\mathcal{M}$ reveals also the properties of many-particle Fock states. For composite particles made of two distinguishable fermions, we have seen in the previous section that $1 - NP \leq \frac{\chi_{N+1}}{\chi_N} \leq 1 - P$. As a consequence, using χ_2 one can estimate other χ_k's and put constraints on the structural parameters λ_k. Note that the value of $\mathcal{M}$ is also related to the condensate fraction $f_{cond} = \langle N|c^\dagger c|N\rangle$ via relation $f_{cond} = N\frac{\chi_N}{\chi_{N-1}}$ as seen previously.

We now see how the measure $\mathcal{M}$ is related to the entanglement between the two constituent fermions of the composite particle. Firstly, we note that in order to evaluate $\mathcal{M}$ for composite particles one does not have to specify g. Since $\mathcal{R} = 2\chi_2 = 2 - 2P$ the measure $\mathcal{M}$ is simply related to the purity as

$$\mathcal{M}(P) = 2 - \frac{3}{3 + 2P(P-2)}. \tag{7.19}$$

It is a continuous monotonically decreasing function of P. In the limit of infinite entanglement the two fermions behave like a boson $\mathcal{M}(0) = 1$. On the other hand, when there is no entanglement the two free fermions evidently exhibit fermionic behavior $\mathcal{M}(1) = -1$. For $0 < P < 1$ the two fermions exhibit either *sub-fermionic* or *sub-bosonic* behavior, depending on the value of the purity. The transition between the two types of behavior for the case of such composite particles in a single mode occurs for $P = \frac{1}{2}$, i.e., for exactly 1 ebit of entanglement, see the lower blue curve in Fig.(7.3). The existence of a critical value of entanglement for the transition between fermionic and bosonic behavior is an important and intuitive result in contrast to the results derived so far [122, 123].

Composite particles of two distinguishable bosons. Let us now discuss the regime $\mathcal{M} > 1$. Consider a system composed of two distinguishable bosons, such as two photons created in a parametric down-conversion process. It is described by similar equations to the system of composite particles of two distinguishable fermions, with $a_k^\dagger$ and $b_k^\dagger$ in (7.15) now being bosonic creation operators, the commutation relation being $[c, c^\dagger] = \mathbb{1} + \Delta$. The optimal

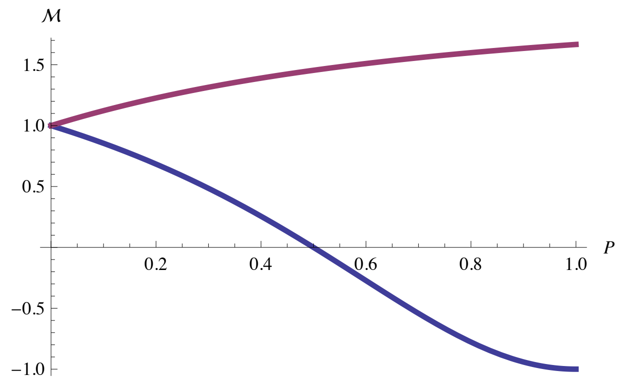

Figure 7.3: The plot of the measure of bosonic quality $\mathcal{M}$ as a function of the purity P for composite particles of two distinguishable bosons (top red curve) and particles made of two distinguishable fermions (bottom blue curve).

channel for addition of these composite particles is also given by (7.17) with the parameter χ_2 defined as

$$\chi_2 = 2\sum_{k\geq l}\lambda_k\lambda_l = \sum_{k,l}\lambda_k\lambda_l + \sum_k \lambda_k^2 = 1 + P. \tag{7.20}$$

In this case, the measure $\mathcal{M}$ is related to the entanglement between the two constituent bosons and is given by

$$\mathcal{M}(P) = 2 - \frac{3}{3 + 2P(P+2)}. \tag{7.21}$$

As in the case of composite particles of two fermions, the value of $\mathcal{M}$ can be used to detect entanglement in the system and to learn structural properties via χ_2. The plot of $\mathcal{M}$ is presented in Fig. (7.3) where the top red curve depicts the behavior of the measure $\mathcal{M}$ as a function of the purity for composite particles made of two distinguishable bosons while the bottom curve depicts this behavior for composite particles made of two distinguishable fermions. It can be seen from the top curve that in the limit of infinite entanglement ($P = 0$) between the two bosons, the system behaves like a true boson $\mathcal{M}(0) = 1$. However, for intermediate values of entanglement ($0 < P \leq 1$), the system exhibits an enhanced bosonic behavior which we term *super-bosonic*. In this regime, the probability of addition of a single composite particle to an already occupied mode is larger than for ideal bosons. The maximal value of $\mathcal{M}(1) = \frac{5}{3}$ occurs for free (non-entangled) bosons.

We now propose an intuitive explanation for the fact that in the limit of large entanglement the value of $\mathcal{M}$ converges to the same point for both the system composed of two bosons and the system composed of two fermions. We start by analyzing the reduced state of the subsystem A in Eq. (7.15). At the moment we do not specify whether we deal with bosons or fermions. The reduced state is given by

$$\rho_A = \sum_k \lambda_k a_k^\dagger |0\rangle\langle 0| a_k.$$

In the limit of small entanglement the distribution $\{\lambda_k\}$ is localized around some k and the subsystem is in a nearly pure state. Its properties are therefore well defined and it can exhibit either fermionic or bosonic behavior, depending on the type of particle. On the other hand, in the limit of large entanglement the distribution $\{\lambda_k\}$ is almost uniform, the state of the subsystem is almost completely mixed and its properties are undefined. Since it can be anywhere in the state-space spanned by all $a_k^\dagger|0\rangle$ it is of little consequence to the system behavior whether the particle is a boson or a fermion. This phenomenon is for example observed in the Hong-Ou-Mandel experiment [131] where one does not observe bunching when the initial state of the two input photons to the beam-splitter is fully random. This explains why in the limit of infinite entanglement systems composed of two bosons and two fermions behave in a similar way (both yielding $\mathcal{M} = 1$). When the entanglement between the constituents is finite, the anti-bunching or bunching of subsystems starts to play a role in the behavior of the total system, resulting in the two regimes $-1 \leq M < 1$ and $M > 1$.

For composite particles made of two distinguishable bosons as the entanglement between the bosons decreases the value of $\mathcal{M}$ increases up to a maximal value of $\frac{5}{3}$. For systems composed of infinitely many bosons $\mathcal{M}$ could reach its maximal value of 2. It would be interesting to investigate if there are any effects in physical phenomena of bosons linked to this regime.

7.4 Two-particle interference

So far, we have considered various ways to characterize bosonic and fermionic behavior, namely via the commutation relation, the formation of a condensate from single particle states, and the effects of addition and subtraction operations. While there is much overlap in the conditions obtained in each case, there are also slight differences suggesting that the bosonic behavior of composite particles depends upon their quantum state and the experimental situation at hand. One common aspect though is that entanglement seems to be necessary for good bosonic behavior in all three scenarios. Another physical situation that one may consider is two-particle interference, where bosonic behavior is captured by the tendency of particles to bunch, while fermionic behavior is related to their tendency to anti-bunch. An interesting question is to quantify the quality of fermionic and bosonic behavior in composite particle systems in these scenarios. In this section following the analysis in [119], we apply addition and subtraction channels to construct a beam splitter for the composite particles and show that the ratio of anti-bunching to bunching probabilities in a two-particle interference experiment also depends on entanglement and that a transition point between fermionic and bosonic behavior exists. Let us now proceed to investigate in detail the properties of composite particles with respect to two-particle interference under the action of beam splitter-like Hamiltonians [131].

Composite particles of two distinguishable fermions. The operator $c_{eff}^{\dagger}$ in (7.17) can be used to construct a beam splitter-like Hamiltonian for composite particles made of two distinguishable fermions as

$$H_{BS} = c_{eff}^{\dagger(1)} c_{eff}^{(2)} + c_{eff}^{\dagger(2)} c_{eff}^{(1)},$$

where superscripts (1) and (2) denote the two beam splitter modes. It is easy to find that a single composite particle in one of the two modes under the action of this Hamiltonian evolves into an even superposition of the two modes in time $t = \frac{\pi}{4}$, irrespective of the χ_2 factor. On the other hand, the evolution of a two-particle state (initally with one particle in each mode) depends on χ_2 as

$$|\psi(t)\rangle = \cos(2\sqrt{\chi_2}t)\,|11\rangle + i\sin(2\sqrt{\chi_2}t)\left(\frac{|20\rangle + |02\rangle}{\sqrt{2}}\right),$$

where the bunched state $(|20\rangle + |02\rangle)/\sqrt{2}$ denotes two composite particles in one mode and the anti-bunched $|11\rangle$ denotes one composite particle in each mode. The probabilities of bunching (p_B) and anti-bunching (p_{AB}) after time $t = \frac{\pi}{4}$ are given as functions of purity $P = 1 - \chi_2$ by

$$p_B = \sin^2\left(\frac{\pi\sqrt{1-P}}{2}\right), \quad p_{AB} = \cos^2\left(\frac{\pi\sqrt{1-P}}{2}\right).$$

For $P = 1$ one observes perfect anti-bunching, whereas for $P = 0$ one observes perfect bunching. The transition between bosonic and fermionic behavior, i.e., $p_B = p_{AB}$ occurs for the critical purity $P = \frac{3}{4}$.

The above example also demonstrates that the notion of bosonic and fermionic quality is not absolute. In fact this quality must be defined with respect to specific physical scenarios. For situations in which particles are added and subtracted to a single mode, the transition from fermionic to bosonic behavior occurs at $P = \frac{1}{2}$, whereas for beam splitter-like situations in which particles are added and subtracted to two modes simultaneously the transition occurs at $P = \frac{3}{4}$. It is possible that for physical situations in which an infinite number of modes can be occupied there is no transition, i.e., the composite particle made of two distinguishable fermions would always behave like a boson.

Composite particles of two distinguishable bosons. One can also consider a beam splitter-like Hamiltonian for composite particles made of two distinguishable bosons. In this case one finds that the probabilities of bunching (p_B) and anti-bunching (p_{AB}) as a function of the entanglement between the two constituent bosons are given by

$$p_B = \sin^2\left(\frac{\pi\sqrt{1+P}}{2}\right), \quad p_{AB} = \cos^2\left(\frac{\pi\sqrt{1+P}}{2}\right).$$

As expected, for all values of P bunching dominates anti-bunching with pure bunching observed at $P = 0$. Moreover, for given entanglement one finds that the composite particle made of two bosons exhibits higher probability of bunching than the composite particle made of two fermions. However, as P increases the probability of anti-bunching increases as well, therefore the particle exhibits sub-bosonic behavior in this test rather than super-bosonic.

7.5 Conclusions and Open Questions

A thorough study has been carried out of the relation between entanglement in the states of composite particles made of two distinguishable fermions or two distinguishable bosons and the quality of bosonic behavior in these systems. An important open question is to identify the states that result in good bosonic and fermionic behavior for composite particles made of multiple fermions. In particular, the role of multipartite entanglement in these systems merits investigation. Based on the considerations of composite particles made of three distinguishable fermions, one may conjecture that in general composite particles of an odd number of fermions always display fermionic behavior, this remains to be proven. For composite particles made of an arbitrary even number of fermions, there are a number of well-known multipartite entanglement classes, it is important to investigate what class of entangled states results in ideal bosonic behavior.

It is known that fermions obey the Fermi-Dirac statistics while bosons obey the Bose-Einstein statistics and classical particles obey the Maxwell-Boltzmann statistics. The analysis in this chapter suggest that a smooth transition between these different statistics may be obeyed by the composite particles. It would be extremely interesting to formulate this transition in statistics as a function of the entanglement in the system. The analysis so far has been restricted to pure states, it needs to be completed for the case of mixed thermal states as well, in general it may be expected that the ground state of composite particles is more entangled than the higher excited states. Addition and subtraction of individual particles has been recently achieved [132] so that developments in this exciting field may find experimental validation in the near future.

Chapter 8

Conclusions

In this thesis, we have examined several unique features of quantum theory such as no-cloning, violation of Bell inequalities, macroscopic local realism, contextuality, and indistinguishable particles from the point of view of the monogamy of correlations in quantum systems. In particular, the central results that we have established can be stated as follows:

- An ansatz solution to the universal cloning problem from 1 to N copies for arbitrary N and arbitrary Hilbert space dimension of the state. The derivation of a monogamy relation for the maximally entangled fraction that must be obeyed by arbitrary qudit states and an illustration of its applicability in condensed matter systems. The demonstration of the solution to symmetric cloning for qubits, its relation with the ground state of the XXZ Hamiltonian on a star configuration, and a derivation of the basic CHSH monogamy relation from asymmetric equatorial 1 to 2 cloning.

- The derivation of monogamy relations for Bell inequality violations in the most common scenario of qubit Bell inequalities with two settings per observer from the correlation complementarity principle. A complete characterization of monogamies for bipartite inequalities was obtained and several tight monogamies for multipartite inequalities were demonstrated.

- A demonstration of the emergence due to monogamy of local realism for correlations in macroscopic systems under the restriction to the set of feasible measurements on these systems.

- An analytic demonstration of the minimal set of measurements required to reveal the contextuality of the simplest contextual system, the qutrit. A proof that all chordal graphs admit joint probability distribution and hence cannot be used for contextuality tests. A derivation of entropic contextual inequalities based on classical properties of the Shannon entropy. A demonstration of the phenomenon of monogamy for contextuality from the no-disturbance principle in analog to the monogamy of Bell inequalities from the no-signaling principle.

- A proof that macroscopically feasible measurements such as magnetization do not yield contexts and that therefore macroscopic systems can be described by a non-contextual theory when the measurements on the system are restricted.

- A study of the role entanglement plays in the bosonic behavior of composite particles made of two distinguishable fermions or bosons. The proposal of a measure for bosonic quality based on the basic probabilistic operations of single particle addition and subtraction. An analysis of the interference from a beam splitter for composite particles and condensation from the viewpoint of local operations.

It is hoped that these results and the open questions listed at the end of each chapter will stimulate further fruitful research.

Bibliography

[1] A. Einstein, B. Podolsky and N. Rosen, Phys. Rev. **47**, 777 (1935).

[2] R. Feynman, Int. J. Theor. Physics **21**, 6-7 (1982).

[3] A. Pais, *"Subtle is the Lord-": The science and the life of Albert Einstein*, (Oxford University Press, 1982).

[4] J. S. Bell, Physics **1**, 195 (1964).

[5] A. K. Ekert, Phys. Rev. Lett. **67**, 661 (1991).

[6] S. Pironio, A. Acín, S. Massar, A. B. de la Giroday, D. N. Matsukevich, P. Maunz, S. Olmschenk, D. Hayes, L. Luo, T. A. Manning and C. Monroe, Nature **464**, 1021 (2010)

[7] G. Brassard, H. Buhrman, N. Linden, A. A. Méthot, A. Tapp and F. Unger, Phys. Rev. Lett. **96**, 250401 (2006).

[8] K. Huang, *Statistical Mechanics*, (Wiley, 1987).

[9] S. Kochen and E. P. Specker, J. Math. Mech. **17**, 59 (1967).

[10] K. Horodecki, M. Horodecki, P. Horodecki, R. Horodecki, M. Pawlowski and M. Bourennane, arXiv/quant-ph: 1006.0468 (2010).

[11] W. K. Wootters and W. H. Zurek, Nature **299**, 802 (1982).

[12] Y. Omar, Int. J. Quant. Inf. **3**, 1 (2005).

[13] N. Gisin, Phys. Lett. A **242**, 1 (1998).

[14] N. Gisin and S. Massar, Phys. Rev. Lett. **79**, 2153 (1997); D. Bruss, A. Ekert and C. Macchiavello, Phys. Rev. Lett. **81**, 2598 (1998).

[15] C. H. Bennett and G. Brassard, Proc. IEEE Int. Conf. on Computers, Systems and Signal Processing, India, 175 (1984).

[16] V. Scarani, S. Iblisdir, N. Gisin and A. Acín, Rev. Mod. Phys. **77**, 1225 (2005).

[17] N. J. Cerf and J. Fiurášek, Progress in Optics **49**, 455 (2006).

[18] V. Bužek and M. Hillery, Phys. Rev. A **54**, 1844 (1996).

[19] D. Bruss, D. P. DiVincenzo, A. Ekert, C. A. Fuchs, C. Macchiavello and J. A. Smolin, Phys. Rev. A **57**, 2368 (1998); M. Keyl and R. F. Werner, J. Math. Phys. **40**, 3283 (1999).

[20] N. J. Cerf, J. Mod. Opt. **47**, 187 (2000); J. Fiurášek, R. Filip and N. J. Cerf, Quant. Inform. Comp. **5**, 583 (2005).

[21] T. Durt, J. Fiurášek and N. J. Cerf, Phys. Rev. A **72**, 052322 (2005).

[22] F. Buscemi, G. M. D'Ariano and C. Macchiavello, Phys. Rev. A **71**, 042327 (2005); C. S. Niu and R. B. Griffiths, Phys. Rev. A **60**, 2764 (1999).

[23] A. Kay, D. Kaszlikowski and R. Ramanathan, Phys. Rev. Lett. **103**, 050501 (2009).

[24] A. Kay, R. Ramanathan and D. Kaszlikowski, arXiv/quant-ph: 1208.5574 (2012).

[25] A. Chandran, D. Kaszlikowski, A. Sen De, U. Sen and V. Vedral, Phys. Rev. Lett. **99**, 170502 (2007).

[26] V. Coffman, J. Kundu and W. K. Wootters, Phys. Rev. A **61**, 052306 (2000).

[27] T. J. Osborne and F. Verstraete, Phys. Rev. Lett. **96**, 220503 (2006).

[28] S. Hill and W. K. Wootters, Phys. Rev. Lett. **78**, 5022 (1997).

[29] C. H. Bennett, G. Brassard, C. Crépeau, R. Jozsa, A. Peres and W. K. Wootters, Phys. Rev. Lett. **70**, 1895 (1993).

[30] A. Jamiołkowski, Rep. Math. Phys. **3**, 275278 (1972).

[31] P. W. Anderson, Phys. Rev. **83**, 1260 (1951).

[32] M. A. Nielsen and I. L. Chuang, *Quantum computation and quantum information*, (Cambridge University Press, 2000)

[33] M. Murao, D. Jonathan, M. B. Plenio and V. Vedral, Phys. Rev. A **59**, 156 (1999).

[34] J. Fiurášek, Phys. Rev. A **64**, 062310 (2001).

[35] M. Horodecki and P. Horodecki, Phys. Rev. A **59**, 4206 (1999).

[36] M. Horodecki, P. Horodecki and R. Horodecki, Phys. Rev. A **60**, 1888 (1999).

[37] S. Iblisdir, A. Acín, N. Gisin, J. Fiurášek, R. Filip and N. J. Cerf, Phys. Rev. A. **72**, 042328 (2005).

[38] R. Tarrach and R. Valentí, Phys. Rev. B **41**, 9611 (1990).

[39] D. Hong-Liang and F. Xi-Ming, Commun. Theor. Phys. **49**, 1353 (2008).

[40] G. M. D'Ariano and C. Macchiavello, Phys. Rev. A **67**, 042306 (2003).

[41] J. F. Clauser, M. A. Horne, A. Shimony and R. A. Holt, Phys. Rev. Lett. **23**, 880 (1969).

[42] B. S. Tsirelson, Lett. Math. Phys. **4**, 93 (1980); R. Horodecki, P. Horodecki and M. Horodecki, Phys. Lett. A **200**, 5 (1995).

[43] V. Scarani and N. Gisin, Phys. Rev. Lett. **87**, 117901 (2001); Phys. Rev. A **65**, 012311 (2001).

[44] B. Toner, Proc. R. Soc. A **465**, 59 (2009).

[45] B. Toner and F. Verstraete, arXiv/quant-ph: 0611001 (2006).

[46] G. M. D'Ariano, C. Macchiavello and P. Perinotti, Phys. Rev. Lett. **95**, 060503 (2005).

[47] N. J. Cerf and S. Iblisdir, Phys. Rev. A **62**, 040301 (2000); S. L. Braunstein, N. J. Cerf, S. Iblisdir, P. v. Loock and S. Massar, Phys. Rev. Lett. **86**, 4938 (2001); J. Fiurášek, Phys. Rev. Lett. **86**, 4942 (2001).

[48] L.- P. Lamoureux, P. Navez, J. Fiurášek and N. J. Cerf, Phys. Rev. A **69**, 040301 (2004); E. Karpov, P. Navez and N. J. Cerf, Phys. Rev. A **72**, 042314 (2005).

[49] A. Fine, Phys. Rev. Lett. **48**, 291 (1982).

[50] D. Collins, N. Gisin, N. Linden, S. Massar and S. Popescu, Phys. Rev. Lett. **88**, 040404 (2002).

[51] S. J. Freedman and J. F. Clauser, Phys. Rev. Lett. **28**, 938 (1972).

[52] A. Aspect, J. Dalibard and G. Roger, Phys. Rev. Lett. **49**, 1804 (1982).

[53] G. Weihs, T. Jennewein, C. Simon, H. Weinfurter and A. Zeilinger, Phys. Rev. Lett. **81**, 5039 (1998).

[54] M. A. Rowe, D. Kielpinski, V. Meyer, C. A. Sackett, W. M. Itano, C. Monroe and D. J. Wineland, Nature **409**, 791 (2001).

[55] R. Werner, Phys. Rev. A **40**, 4277 (1989).

[56] M. Pawlowski, Phys. Rev. A **82**, 032313 (2010); J. Barrett , L. Hardy and A. Kent, Phys. Rev. Lett. **95**, 010503 (2005).

[57] Ll. Masanes, A. Acín and N. Gisin, Phys. Rev. A **73**, 012112 (2006).

[58] M. Pawłowski and Č. Brukner, Phys. Rev. Lett. **102**, 030403 (2009).

[59] P. Kurzynski, T. Paterek, R. Ramanathan, W. Laskowski and D. Kaszlikowski, Phys. Rev. Lett. **106**, 180402 (2011).

[60] G. Tóth and O. Gühne, Phys. Rev. A **72**, 022340 (2005).

[61] S. Wehner and A. Winter, J. Math. Phys. **49**, 062105 (2008); New J. Phys. **12**, 025009 (2010).

[62] G. V. Steeg and S. Wehner, Quant. Inf. and Comp. **9**, 801 (2009).

[63] M. Żukowski and Č. Brukner, Phys. Rev. Lett. **88**, 210401 (2002).

[64] W. Laskowski, T. Paterek, M. Żukowski and Č. Brukner, Phys. Rev. Lett. **93**, 200401 (2004).

[65] J. Oppenheim and S. Wehner, Science **330**, 1072 (2010).

[66] N. D. Mermin, Phys. Rev. Lett. **65**, 1838 (1990).

[67] J. M. Aldous and R. J. Wilson, *Graphs and Applications: an Introductory Approach*, (Undergraduate Mathematics Series, Springer-Verlag, 2000).

[68] M. Pawłowski, T. Paterek, D. Kaszlikowski, V. Scarani, A. Winter and M. Żukowski, Nature **461**, 1101 (2009).

[69] A. Aspect, P. Grangier and G. Roger, Phys. Rev. Lett. **47**, 460 (1981).

[70] A. Aspect, Nature **398**, 189 (1999).

[71] P. Grangier, Nature **409**, 774 (2001).

[72] F. Károlyházy, Il Nuovo Cimento A **42**, 390(1966).

[73] I. C. Percival, Proc. R. Soc. A **451**, 503 (1995).

[74] P. Pearle and E. Squires, Found. Phys. **26**, 291 (1996).

[75] L. Diósi, Phys. Lett. A **105**, 199 (1984); Phys. Lett. A **120**, 377 (1987); Phys. Rev. A **40**, 1165 (1988).

[76] R. Penrose, Gen. Relativ. Gravit. **28**, 581 (1996); Phil. Trans. R. Soc. A **356**, 1927 (1998); *The Road To Reality*, (Jonathan Cape Publishers, London, 2004).

[77] G. C. Ghirardi, A. Rimini and T. Weber, Phys. Rev. D **34**, 470 (1986).

[78] W. H. Zurek, Phys. Today **44**, 36 (1991).

[79] W. H. Zurek, Rev. Mod. Phys. **75**, 715 (2003).

[80] M. Schlosshauer, *Decoherence and the quantum-to-classical transition*, (Springer, 2007).

[81] A. Peres, *Quantum Theory: Concepts and Methods*, (Kluwer Academic, 1995).

[82] P. Busch, M. Grabowski and P. J. Lahti, *Operational Quantum Physics*, (Springer, New York, 1995).

[83] D. Poulin, Phys. Rev. A **71**, 022102 (2005).

[84] J. Kofler and Č. Brukner, Phys. Rev. Lett. **99**, 180403 (2007); Phys. Rev. Lett. **101**, 090403 (2008); arXiv/quant-ph:1009.2654 (2010).

[85] L. M. K. Vandersypen, M. Steffen, G. Breyta, C. S. Yannoni, M. H. Sherwood and I. L. Chuang, Nature **414**, 883 (2001).

[86] P. Davies, *Randomness and Complexity. From Leibniz to Chaitin*, (World Scientific, Singapore, 2007); J. Kofler and Č. Brukner, arXiv/quant-ph:1009.2654 (2010).

[87] B. Julsgaard, A. Kozhekin and E. S. Polzik, Nature **413**, 400 (2001).

[88] B. M. Terhal, A. C. Doherty, and D. Schwab, Phys. Rev. Lett. **90**, 157903 (2003).

[89] R. Ramanathan, T. Paterek, A. Kay, P. Kurzynski and D. Kaszlikowski, Phys. Rev. Lett. **107**, 060405 (2011).

[90] N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, (Harcourt, Orlando, 1976).

[91] L. E. Sadler, J. M. Higbie, S. R. Leslie, M. Vengalattore and D. M. Stamper-Kurn, Nature **443**, 312 (2006); K. Jensen, W. Wasilewski, H. Krauter, T. Fernholz, B. M. Nielsen, A. Serafini, M. Owari, M. B. Plenio, M. M. Wolf and E. S. Polzik, Nature Phys. **7**, 13 (2011).

[92] M. Navascues and H. Wunderlich, Proc. Roy. Soc. Lond. A **466**, 881 (2009).

[93] D. Collins and N. Gisin, J. Phys. A **37**, 1775 (2004); M. Froissart, Nuov. Cim. B **64**, 241 (1981); C. Śliwa, Phys. Lett. A **317**, 165 (2003).

[94] A. Acín, N. Gisin and B. Toner Phys. Rev. A **73**, 062105 (2006).

[95] A. Tonge, technical report TR/08/83, "Low Dimensional Grothendieck constants" (1983).

[96] J. Barrett, Phys. Rev. A **65**, 042302 (2002).

[97] R. W. Spekkens, D. H. Buzacott, A. J. Keehn, B. Toner and G. J. Pryde, Phys. Rev. Lett. **102**, 010401 (2009).

[98] A. A. Klyachko, M. A. Can, S. Binicoğlu and A. S. Shumovsky, Phys. Rev. Lett. **101**, 020403 (2008).

[99] R. Lapkiewicz, P. Li, C. Schaeff, N. K. Langford, S. Ramelow, M. Wieśniak and A. Zeilinger, Nature **474**, 490 (2011).

[100] S. L. Braunstein and C. M. Caves, Phys. Rev. Lett. **61**, 662 (1988).

[101] M. Żukowski and Č. Brukner, Phys. Rev. Lett. **88**, 210401 (2002).

[102] A. Cabello, S. Severini and A. Winter, arXiv/quant-ph: 1010.2163 (2010).

[103] T. Fritz and R. Chaves, arXiv:quant-ph: 1112.4788 (2011); R. Chaves and T. Fritz, Phys. Rev. A **85**, 032113 (2012).

[104] P. Kurzynski, R. Ramanathan and D. Kaszlikowski, Phys. Rev. Lett. **109**, 020404 (2012).

[105] R. Ramanathan, A. Soeda, P. Kurzynski and D. Kaszlikowski, Phys. Rev. Lett. **109**, 050404 (2012).

[106] M. Sadiq, P. Badziag, M. Bourennane and A. Cabello, arXiv/quant-ph: 1106.4754 (2011).

[107] S. Yu and C. H. Oh, Phys. Rev. Lett. **108**, 030402 (2012).

[108] C. Berge, Math.-Nature Reihe **10**, 114 (1961).

[109] L. Lovász, Disc. Math. **2**, 253 (1972).

[110] S. Popescu and D.Rohrlich, Found. of Phys. **24**, 379 (1994).

[111] P. Kurzynski, A. Soeda, R. Ramanathan, A. Grudka, J. Thompson and D. Kaszlikowski, arXiv/quant-ph: 1111.2696 (2011).

[112] A. R. Swift and R. Wright, J. Math. Phys. **21**, 77 (1980).

[113] A. M. Gleason, J. Math. Mech. **6**, 885 (1957).

[114] N. D. Mermin, Rev. Mod. Phys. **65**, 803 (1993).

[115] R. W. Spekkens, Phys. Rev. A **75**, 032110 (2007).

[116] A. Cabello, Phys. Rev. Lett. **90**, 190401 (2003); A. Grudka and P. Kurzynski, Phys. Rev. Lett. **100**, 160401 (2008).

[117] I. Duck and E. C. G. Sudarshan, *Pauli and the Spin-Statistics Theorem*, (World Scientific, Singapore, 1997).

[118] R. Ramanathan, P. Kurzynski, T. K. Chuan, M. F. Santos and D. Kaszlikowski, Phys. Rev. A (Brief Reports) **84**, 034304 (2011).

[119] P. Kurzynski, R. Ramanathan, A. Soeda, T. K. Chuan and D. Kaszlikowski, New Journ. of Phys. **14**, 093047 (2012).

[120] ed. A. Griffin, D. W. Snoke and S. Stringari, *Bose-Einstein Condensation*, (Cambridge University Press, 1995).

[121] M. Combescot and C. Tanguy, Europhys. Lett. **55**, 390 (2001).

[122] C. K. Law, Phys. Rev. A **71**, 034306 (2005).

[123] C. Chudzicki, O. Oke and W. K. Wootters, Phys. Rev. Lett. **104**, 070402 (2010).

[124] E. Schmidt, Math. Annalen. **63**, 433 (1906);

[125] L. E. Dickson, *Elementary Theory of Equations*, (Wiley & Sons, 1914).

[126] M. Combescot, O. Betbeder-Matibet and F. Dubin, Phys. Rep. **463**, 215 (2008).

[127] M. A. Nielsen, Phys. Rev. Lett. **83**, 436 (1999).

[128] C. Comte and P. Nozières, J. Physique France **43**, (7) 1069 (1982); S. Rombouts *et. al.*, Mod. Phys. Lett. A **17**, 1899 (2002); S. Rombouts *et. al.*, Europhys. Lett. **63**, 785 (2003).

[129] P. Nozières and C. Comte, J. Physique France **43**, (7) 1083 (1982).

[130] A.W. Marshall and I. Olkin, *Inequalities: Theory of Majorization and Its Applications*, (Academic Press, California, 1979).

[131] C. K. Hong, Z. Y. Ou and L. Mandel, Phys. Rev. Lett. **59**, 2044 (1987).

[132] V. Parigi, A. Zavatta, M. S. Kim and M. Bellini, Science **317**, 1890 (2007); A. Zavatta, V. Parigi, M. S. Kim, H. Jeong and M. Bellini, Phys. Rev. Lett. **103**, 140406 (2009).