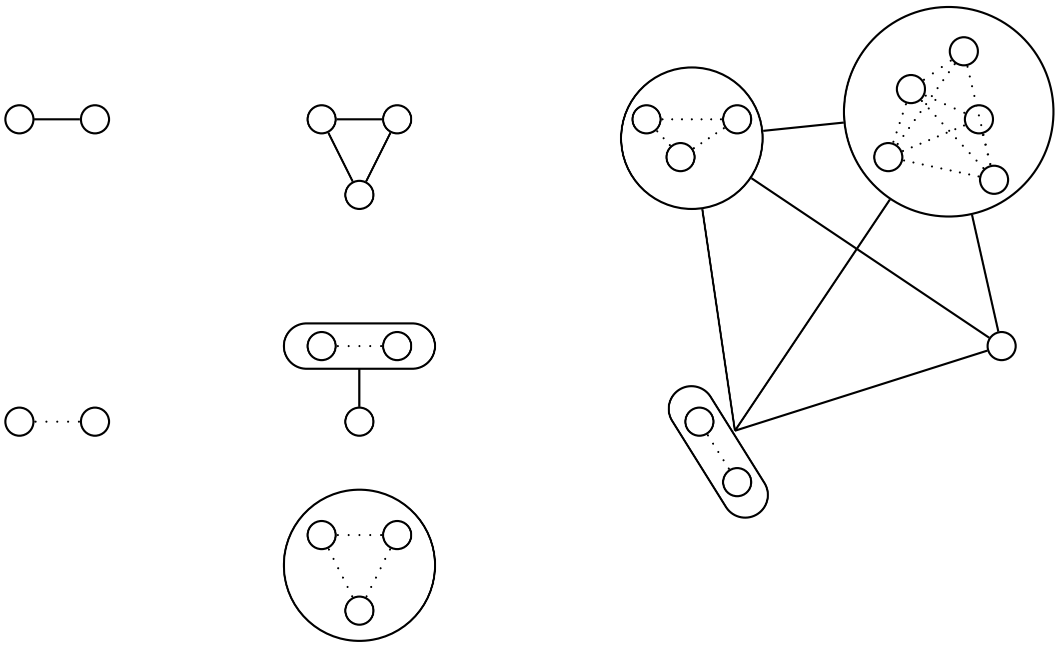
Entanglement, Local Hidden Variables and Bell-inequalities

An investigation in multi-partite quantum mechanics.



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Masters Thesis in the Foundations of Physics,
University of Utrecht, June 2002.

Preface

I would like to thank Jos Uffink for his willingness to help, very careful reading and great suggestions. Thanks to Joris Mooij and Luc Bouten for our discussions about physics and humour. Special thanks to Jochem, Maarten, Saskia, Peter and my parents. Your love must be infinite.

■ Notes:

(i) Part of this thesis is published together with George Svetlichny (see Ref. [92]) and with Jos Uffink (see Ref. [93]).

(ii) Most of the here presented work is a discussion of already published work by others. I claim no originality for the content nor for the terminology except for the work in the articles mentioned above and for providing a red thread to unify the fragmentated results already existing out there in the literature.

Contents

Chapter 1

Introduction

It is well-known that the question whether a local hidden variables theory can exist for quantum mechanics was answered in the negative by John Bell in 1964. He derived the nowadays called Bell-inequalities obeyed by any local hidden variables theory and showed in his Bell-theorem that quantum mechanics would violate these inequalities [20]. Bell used a particular pure bi-partite entangled quantum state, the so-called singlet state of two spin-1/2 particles. And he was not the only one. All variations on the same theme –i.e. quantum mechanical violation of certain Bell-inequalities– that had appeared in the Sixties, Seventies and early Eighties used such bi-partite pure entangled states. It turned out that all these states allow for violation of Bell-inequalities and could therefore not be modeled by a local hidden variables model. As a consequence entanglement was identified with non-locality; all entangled states were thought to be non-simulable by a local hidden variables model. However, this widespread belief has been shown not to be true.

In 1989 Werner [65] showed that certain bi-partite mixed states have a local hidden variables model for all projective measurements despite being entangled. Subsequently, through the study of mixed quantum states and the extension to multi-partite Bell-type inequalities, it was slowly realized that entanglement and violation of Bell-type inequalities (i.e. factorisability (of local hidden variable predictions) and separability (of quantum states) are quite distinct notions that cannot be identified, except for the special case of pure two-particle states. This realisation is the starting point for this thesis and is captured in the following remark:.

> *Whereas in the late Eighties there was hardly any difference between entangled states and states violating a Bell inequality, we have a much more subtle discrimination nowadays.* R. Werner [105] (2001).

Thus there are two issues which are quite separate:

1. Which states are entangled?

2. Which states have non-local characteristics?

Their status is the following. The first question asks about the *mathematical structure* of quantum mechanics . By definition any state which cannot be written as a direct-product or as a mixture of direct products is called 'entangled'. The definition gives no problems. There are only practical problems: It is very difficult to determine if an unknown state can be written as a mixture of direct product states or not. The second question asks about the *physical structure* of hidden variables theories. The point is that it is not at all obvious what locality actually entails and whether all entangled states have non-local characteristics.

Answering the first question requires an analysis of the quantum mechanical state space and the second an analysis of simulability through local hidden variables theories. In this thesis both analyses will be discussed. In other words, local hidden variable theories will be used as a means for investigating quantum mechanics and *vice versa*. For both hidden variable theories and the feature of entanglement an discussion of the multi-partite extension for pure and mixed states is given.

This allows for the following question to be answered. What is the argument for taking an entangled state to intrinsically possess non-local (as opposed to merely entangled) correlations? This question "When is a quantum state local?" has the obvious answer that a quantum state is local if a local HV-theory exists which is valid for all results of all possible local actions. Or equivalently, a quantum state is local when it cannot be made to violate any Bell-type inequality that is obtained from a local hidden variables theory. Although this answer is very simple, its constituents are not. For what are these Bell-type inequalities? And what are these local hidden variable theories? Subsequently, exactly which quantum states are non-local? These questions will be explored throughout this thesis by discussing the currently known results and by adding some new ideas and results.

1.1 Structure of this Thesis

In a nutshell each chapter in this thesis can be characterised as follows. Chapter 2 deals with the basic mathematical structure of quantum mechanics. Chapter 3 is devoted to multi-partite entanglement and related quantum mechanical features. Chapter 4 treats multi-partite local hidden variable theories and Bell-type inequalities for full and partial factorisability. Chapter 5 addresses the connections and relations between chapter 3 and 4. Finally chapter 6 treats a preliminary extension of the previous chapters from orthodox quantum measurements to more general measurements.

To further introduce this thesis I will give a short overview of each chapter. As preliminary information the mathematical structure of quantum mechanics is presented in chapter 2. Three different sets of postulates are discussed. The first for pure states and projective measurements, the second for the extension to mixed states, and the third for the extension of orthodox measurements given by projection valued measures (PVM) to generalized measurements given by positive operator valued measures (POVM).

I give the standard formulation of measurement compatibility (i.e. simultaneous measurability) of observables. In this standard account measurement compatibility is identified with commutativity of the operators that correspond to the observables. However, I criticize this identification and argue that commutativity is not sufficient for measurement compatibility using a simple example that was inspired by Harvey Brown [82].

In chapter 3 I consider quantum entanglement. An entangled state is defined as a non-separable state. Therefore the separability properties of density operators are discussed. The partial transpose criterium is discussed and shown to give a necessary criterium for separability, and for small Hilbert spaces a sufficient criterium as well. The structure of the bi-partite, tri-partite and N-partite entangled state space is investigated and specific distinctions such as maximal and full entanglement are obtained. Further, I discuss the phenomenon of distillability of a collection of entangled states to one or more maximally entangled bi-partite states.

In order to confront quantum mechanics and the feature of entanglement to the structure of hidden variables theories, I discuss in chapter 4 the incompleteness problem of quantum mechanics. The discussion of this problem –whether or not quantum mechanics provides a complete physical theory– serves as a stepping stone for the study of hidden variable theories as theories that could possibly be more complete than quantum mechanics itself. These are required to reproduce quantum mechanics (this requirement is called the Quantum-criterium) and further to obey a specific locality hypothesis that entails factorisability.

These local hidden variables theories give rise to the Bell-inequality and the Bell-theorem. The derivation of both is presented as preliminary work for the remainder of the thesis. In this remainder more complex systems are studied than the bi-partite spin-1/2 systems which are the paradigmatic systems for the original Bell-theorem and all its initial variations on the same theme.

In section 4.3 I discuss recent *Gedankenexperiments* obtained by considering more complex bi- and tri-partite systems. These are the so-called Bell-theorems without inequalities and the algebraic theorems. As examples the Bell-theorem without inequalities of Hardy and the algebraic theorem of Greenberger, Horne and Zeilinger (GHZ) are discussed. These recent Bell-theorems are compared to the original Bell-theorem for logical strength and experimental testability.

The extension to N-partite systems results in the necessary distinction between the specific locality-hypotheses of full and partial factorisability. The Bell-Klyshko N-partite Bell-type inequalities for full factorisability are presented and furthermore they are extended to complete sets (i.e. necessary and sufficient sets) of Bell-type inequalities for local realism to hold. The extension to multi-partite systems for which the specific locality hypothesis of partial factorisability is required to hold, gives a new type of hidden variable theories, the so-called partial local hidden variables theories. The so-called generalized Svetlichny inequalities are derived and shown to be necessary inequalities for any such theories to hold.

The three types of inequalities – the Bell-inequalities, the N-partite Bell-Klyshko inequalities for full separability and the Svetlichny inequalities for partial separability – are all confronted with the feature of quantum entanglement. I show that these inequalities give experimentally accessible sufficient conditions for respectively bi-partite and full N-partite entanglement. These inequalities thus serve a dual purpose. As tests of certain hidden variables theories and as tests for entanglement.

In order to further investigate the quantum mechanical state space by means of local hidden variable theories, chapter 5 is largely devoted to quantum mechanical violations and non-violations of the Bell-type inequalities for full factorisability and the Svetlichny inequalities for partial factorisability. The following two central questions are discussed:

1. What is the set of states violating a Bell-type inequality?
2. What states give maximal violations?

The discussion for the case of full factorisability, i.e. (non-)violations of Bell-type inequalities, has been performed for all possible systems (M sub-systems with arbitrary Hilbert spaces each) and for all measurement configurations (N observers with m d-valued observables, notated as (N, M, d)). In contrast,(non-) violations for the case of partial factorisability are only presented for the single measurement configuration $(N, 2, 2)$.

Noteworthy is the fact that the fully separable states are not the only states non-violating any Bell-type inequality. Some entangled states exist that have a local HV-model for all orthodox measurements and will thus not violate a Bell inequality. This entanglement can not be revealed using a Bell inequality when subjected to orthodox measurements. It is therefore said to be 'hidden entanglement'. But surprisingly it can be revealed using a Bell inequality when performing generalized quantum measurements such as sequential measurements that can be modeled using POVMs. This the so-called phenomenon of 'revealing hidden entanglement'. It has broadened the class of quantum states that have statistical properties that violate local realism.

Three examples of revealing hidden non-locality –using sequential, filtering and collective measurements– motivates the discussion of chapter 6 of local hidden variables theories for more general types of measurement than the orthodox. In order to apply the hidden variables formalism to these general quantum measurements, the Quantum-criterium is changed: the local hidden variables model has to reproduce not only the orthodox measurements but also the specific types of general measurements such as sequential measurements, POVM measurements and the extension to to local actions and classical communication (LOCC) and to collective measurements. Because not many results are known, the discussion in the last chapter stays rather conceptual and is not very in depth.

Throughout this thesis the investigation of quantum mechanics using local hidden variables theories results in a classification of different quantum states. This classification is presented at the end of chapter 2, 3, 4 and 5 and is performed (i) through the formalism, (ii) through extending the formalism, (iii) through entanglement properties and aspects of quantum information, (iv) through factorisability (full and partial) and hidden variables simulability, (v) through (non)-violations of Bell-type inequalities.

A mathematical appendix is included for background information about the theory of operators on a (tensor product) Hilbert space. Finally, a list of abbreviations is given for convenience.

Chapter 2

Quantum mechanical Preliminaries

2.1 Introduction

Initially quantum mechanics was developed to describe the world of atoms and in particular to explain the observed spectral lines in spectrometers. During the development of quantum mechanics, through the early theories of Niels Bohr and finally in 1926 culminating in the work of Heisenberg and subsequently of Schrödinger, it eventually became clear that quantum mechanics is primarily a mathematical theory describing measurement outcomes rather than some underlying physical processes.

Asking a group of physicists "What is quantum mechanics all about?"[51] will no doubt generate a multitude of different answers. In this chapter I try to present what I believe almost all physicists are willing to accept as the basic structure of quantum mechanics. I will present a summary of the mathematical and physical structure of quantum mechanics needed to set the terminology and provide basic tools and concepts for the rest of the treatise. It does not contain new results; this summary is a compilation of the texts of Isham [45], Redhead [46] and especially of Hilgevoord *et al.* [47].

This chapter is organized as follows. First, in section 2.2 I will present the postulates for the orthodox formalism of quantum mechanics for pure states. I will then discuss in section 2.3 the extension to mixed states and composite systems. This leads to a second set of postulates for orthodox quantum mechanics for all possible states, both pure and mixed. The mixed state formalism gives rise to a first classification of the quantum mechanical state space. This is given in section 2.6. In the next section I will treat orthodox measurement theory and its extension to the so-called general measurements using projection operator valued measures. This leads to the third set of postulates of quantum mechanics, i.e. for the quantum formalism using these general measurements. Finally, this chapter ends in section 2.8 with the standard formulation of measurement compatibility, supplemented with a critique of this standard account.

2.2 Postulates of Orthodox Quantum Mechanics for Pure States

The formalism of quantum mechanics (QM) is designed to account for two features of microscopic systems. Firstly, the possible results of measuring certain physical magnitudes are confined to a restricted set of values. Secondly, it is in general not possible to predict for any physical magnitude which is being measured what value will turn up, only the *probability* that any particular value will turn up. In order to account for these features, quantum mechanics represents measurable physical magnitudes, called observables, by self-adjoint operators on a Hilbert space. Furthermore, the system is assigned a state which is an expression of the various probabilities, for all observables, of the possible outcomes of the experiment.

These physical concepts of state, observable and measurement outcome are related to the mathematical structure[1] of QM by the following von Neumann postulates in the conventional Dirac bracket notation:

1. *States (pure case).* To every physical system corresponds a Hilbert space $\mathcal{H}$ which is the state space; the states correspond bijectively to unit vectors $|\,\psi\rangle$ in $\mathcal{H}$ – apart from an irrelevant global fase factor $e^{i\theta}$ ($\theta \in \mathbb{R}$)– and equivalently to the one dimensional projection operators $P_\psi = |\,\psi\rangle\,\langle\,\psi|$. The state space of a composed physical system is the direct product space of the state spaces of the subsystems.

2. *Observables-postulate.* To every physical quantity or observable $\mathcal{A}$ corresponds a self-adjoint operator A acting on $\mathcal{H}$.

3. *Spectrum-postulate.* The only possible outcomes of a measurement of observable $\mathcal{A}$ corresponding to the operator A are the values of the spectrum of A. This is also called the Quantisation Algorithm [46].

4. *Born rule (discrete case).* For a system in the state $|\,\psi\rangle \in \mathcal{H}$ ($\dim \mathcal{H} = N$), upon measurement of observable $\mathcal{A}$ (represented by the operator A) with a discrete spectrum, the probability for the measurement to yield the outcome a_i (with n_i-fold degeneracy) is equal to

$$\begin{aligned} \mathrm{Prob}^{|\,\psi\rangle}(a_i) &= \sum_{j=1}^{n_i} |\,\langle\, a_i, j|\,\psi\rangle|^2 \\ &= \langle\,\psi|\,P_{a_i}\,|\,\psi\rangle = Tr\,[P_{|\,\psi\rangle}P_{a_i}] \end{aligned} \tag{2.1}$$

where $P_{|\,\psi\rangle} = |\,\psi\rangle\,\langle\,\psi|$ and $P_{a_i} = \sum_{j=1}^{n_i} |\,a_i, j\rangle\,\langle\,a_i, j|$. The expectation value of A in the state $|\,\psi\rangle$ then yields

$$\langle A\rangle_{|\,\psi\rangle} = \sum_{i=1}^{N}\sum_{j=1}^{n_i} a_i|\,\langle\, a_i, j|\,\psi\rangle|^2 = \langle\,\psi|\,A\,|\,\psi\rangle = Tr\,[AP_{|\,\psi\rangle}] \tag{2.2}$$

This is also called the Statistical Algorithm [46].

[1] See appendix A for a detailed summary of the mathematical formalism of complex vector spaces.

5. *Schrödinger-postulate.* The state of a system upon which no measurements are made during a certain time interval, will evolve according to the following unitary transformation:

$$|\,\psi(t+dt)\rangle = U(t,t+dt)\,|\,\psi(t)\rangle = \exp[-iHdt/\hbar]\,|\,\psi(t)\rangle\,. \tag{2.3}$$

In infinitesimal form this is equal to the Schrödinger equation that governs the time evolution of a state $|\,\psi(t)\rangle$ under the influence of a Hamiltonian operator H:

$$i\hbar\frac{d}{dt}\,|\,\psi(t)\rangle = H\,|\,\psi(t)\rangle\,. \tag{2.4}$$

6. *Projection-postulate.* If a measurement is performed on a physical system in the state $|\,\psi\rangle$ of the operator A corresponding to the observable $\mathcal{A}$, and the result is the eigenvalue a_i of the spectrum of A, then the reduced state directly after the measurement will be the following:

$$|\,\psi\rangle \rightsquigarrow \frac{P_{a_i}\,|\,\psi\rangle}{\|P_{a_i}\,|\,\psi\rangle\,\|}. \tag{2.5}$$

Depending upon the degeneracy of A the projection operator P_{a_i} need not be one-dimensional[2]. If the operator A is maximal (i.e. non-degenerate) the state 'collapses' to the unique eigenstate $|\,a_i\rangle$ because in this case P_{a_i} is a one-dimensional projection operator. Note that this evolution is in general not a unitary evolution and thus that this postulate introduces a *second* sort of dynamics which is *not* governed by the Schrödinger evolution.[3]

The first four postulates translate the physical concepts of system, state and observable into mathematical concepts, the last two postulates describe the two different time evolutions of states [47]. I will not explicitly comment here any further on these postulates even though very much can be said at this moment, but throughout this chapter I will discuss more implications and details.

2.3 Pure and Mixed States

The above mentioned postulates hold only for *pure states*, i.e. for state vectors $|\,\psi\rangle$ in $\mathcal{H}$. However, not all systems can be represented as a pure state and thus we want to be able to treat mixtures of pure states as well. Therefore I will follow the analogue of classical mixed states, by considering probability distributions on the set of state vectors in $\mathcal{H}$. Physical states will now correspond in a bijective way to probability measures on *subspaces* of $\mathcal{H}$. There are different ways of presenting the mixed state formalism. I will follow the approach of Ref. [47].

[2]Von Neumann originally proposed this postulate with all the P_{a_i} one-dimensional; he proposed the evolution $|\,\psi\rangle \rightsquigarrow |\,a_i\rangle$. Lüders generalized this in 1951 to also include projections not just onto particular eigenvectors but to whole eigenspaces. He thus proposed the 'collapse' as given in Eq.(2.5).

[3]Some people do not accept this postulate for it gives rise to the so called Measurement Problem. They want to account for the measurement process using only the unitary evolution of the Schrödinger Postulate. See also footnote 6. However the Measurement Problem will not be dealt with here.

In order to hold on to the structure of $\mathcal{H}$ we will consider not arbitrary subsets of $\mathcal{H}$ but the set $\mathcal{P}(\mathcal{H})$ of all subspaces of $\mathcal{H}$ generated by the orthogonal projection operators. This means that attention is focussed on the projection operators that project onto these subspaces. Now, we want a probability measure μ defined on the set $\mathcal{P}(\mathcal{H})$, i.e. a map μ: $\mathcal{P}(\mathcal{H}) \to [0,1]$ with the following two requirements. First an additivity requirement. The measure that is given to a direct sum of projection operators must be equal to the sum of the individual measures given to each projection operator itself. Thus, suppose $\{P_1, P_2, \ldots, P_N\}$ is a set of orthogonal projection operators ($P_i \perp P_j$, $\forall i \neq j$), then

$$\mu\left(\bigoplus_{j=1}^{N} P_j\right) = \sum_{j=1}^{N} \mu(P_j). \tag{2.6}$$

The second, obvious, requirement is that the measure given to the zero-space is 0 and to the full space is 1, i.e.

$$\mu(0) = 0 \text{ and } \mu(\mathbb{1}) = 1. \tag{2.7}$$

Equations (2.6) and (2.7) are a minimal set of requirements on any quantum probability function μ [47].

The following question now arises: What are the possible probability measures $\mu(P)$ definable over the set $\mathcal{P}(\mathcal{H})$ of a Hilbert space? Gleason answered this question in 1957 by proving the following theorem [22]:

Theorem 2.3.1 (Gleason). *For dim $\mathcal{H} > 2$ every probability measure μ on $\mathcal{P}(\mathcal{H})$ is of the form*

$$\mu(P) = \mathrm{Tr}[P\rho]. \tag{2.8}$$

Here ρ is a self-adjoint, positive operator with trace equal to 1:

$$\begin{array}{ll} (i) & \rho = \rho^\dagger \\ (ii) & \langle \psi | \rho | \psi \rangle \geq 0 \,, \quad \forall \,| \psi \rangle \in \mathcal{H} \\ (iii) & \mathrm{Tr}[\rho] = 1. \end{array} \tag{2.9}$$

The proof will not be given here but can be found in Ref. [22]. Gleason has thus proved the remarkable result that the *only* way of satisfying Eq. (2.6) and (2.7) is with the aid of an operator ρ and the measure of Eq.(2.8).[4]

The operator ρ is known as the *density operator* or the *statistical operator*. In analogy with classical mixtures, ρ is called the state of a physical system, i.e. each state is represented by a unique self-adjoint positive operator. The density operators form a *convex set* notated as $\mathcal{S}$, i.e. for ρ_1 and ρ_2 being density operators, then $\alpha\rho_1 + \beta\rho_2$ where α, $\beta \in [0,1]$ and $\alpha + \beta = 1$ is again a density operator.

How does this density operator ρ relate to the one dimensional projection operators P_ψ that correspond to the pure states $|\,\psi\rangle$? To answer this question we state the following theorem which will not be proved here.

[4] An important corollary which gave rise to the Kochen-Specker theorem prohibiting non-contextual hidden variable models, is the fact that for dim $\mathcal{H} > 2$ the measure $\mu(P)$ is *continuous* in P: $\mu(P) = \mu(P')$ for $P \to P'$. Thus some probability measures on $\mathcal{H}$ are ruled out on the basis of Gleason's theorem, *simply because they are discontinuous.* Gleason's theorem places strong constraints on any attempts to modify the standard quantum formalism, as might be desired by the construction of hidden variables (see chapter 4).

Theorem 2.3.2. *The one-dimensional projection operators in $\mathcal{P}(\mathcal{H})$ are the extreme elements of the convex set $\mathcal{S}$ of all density operators on $\mathcal{H}$.* (For proof see [47].)

From this theorem it thus follows that (i) because P_ψ is an extreme element, it cannot be decomposed in the form $P_\psi = \alpha\rho_1 + (1-\alpha)\rho_2$ where $\alpha \in (0,1)$ and furthermore that (ii) the one-dimensional projection operators are the *only* extreme elements.

Any finite N-dimensional density operator ρ is bounded and self-adjoint and from the spectral theorem (see appendix B) it has a complete and orthonormal set of eigenstates $|\,\alpha_i\rangle$. (Where for simplicity we have taken ρ to be non-degenerate). An arbitrary $\rho \in \mathcal{S}(\mathcal{H})$ can thus be written as:

$$\rho = \sum_{i=1}^{N} \alpha_i \rho_i, \qquad \text{with} \qquad \rho_i = |\,\alpha_i\rangle\,\langle\,\alpha_i| \in \mathcal{P}(\mathcal{H}), \tag{2.10}$$

where $\alpha_i \in [0,1]$ and $\sum_{i=1}^{N} \alpha_i = 0$. This follows from $\alpha_i = \langle\,\alpha_i|\,\rho\,|\,\alpha_i\rangle \geq 1$ and from $Tr[\rho] = \sum_{i=1}^{N} \alpha_i = 1$. Eq.(2.10) is thus a convex decomposition of ρ in terms of projection operators. ρ is an extreme element iff the sum in Eq.(2.10) reduces to one term, in which case it is a one-dimensional projection operator.

A physical state that can be represented as a one-dimensional projection operator is called a *pure state*. A state ρ which can be decomposed into a convex combination of projection operators is called a *mixed state* or *mixture*.

2.4 Mixed states and Composite Systems

2.4.1 Interpretation of Mixed States: Single Systems

In the previous section 2.3 we introduced the mixed states in a formal and rather abstract way. But apart from this strict formalism, what can we think a mixed state represents? A mixture of physical systems in certain well-defined states, just like in the classical formalism? No, as will be shown, this naive interpretation has unsurmountable problems.

However, the spectral decomposition of Eq.(2.10) is suggestive of the just mentioned interpretation in terms of a classical mixture. For it is the case that according to Eq.(2.10) a state ρ corresponds to a probability measure on the eigenvectors $|\,\alpha_i\rangle$ that assigns a probability α_i to $|\,\alpha_i\rangle$: $\mu_\rho(\rho_i) = \mathrm{Tr}[\rho_i\rho] = \mathrm{Tr}[\alpha_i\rho_i] = \alpha_i\mathrm{Tr}[\rho_i] = \alpha_i$. Then the expectation value of an operator A in the state ρ is equal to $\langle A\rangle = \mathrm{Tr}[A\rho]$, which reads in the spectral decomposition of Eq.(2.10):

$$\langle A\rangle = \sum_{i=1}^{N} \alpha_i \mathrm{Tr}[A\rho_i] = \sum_{i=1}^{N} \alpha_i \,\langle\,\alpha_i|\,A\,|\,\alpha_i\rangle\,. \tag{2.11}$$

This is the weighted sum of the expectation values of A in the states $|\,\alpha_i\rangle$ each with weights α_i. This indeed suggests that the mixed state ρ is a mixture of physical systems each, *being in reality*, in the pure states $|\,\alpha_i\rangle$ with fraction α_i. This is correct if one explicitly prepares the ensemble by mixing the systems prepared in the pure states $|\alpha_i\rangle$ in the right relative fractions α_i. This is analogous to classical statistical mechanics and it was the original motivation for Von Neumann to introduce the density operators[5]. In conclusion, the density operators admit by construction the interpretation that each system of the ensemble is *in reality* described by one of the state vectors $|\alpha_i\rangle$, but we do not know which one, and that α_i merely is the probability for this state to occur.

However this so-called *'ignorance interpretation'* of the density operator ρ has problematic consequences, which I will show using the formulation of Ref. [47]. The problem is that the choice of basis vectors in Eq.(2.10) is non-unique. Thus ρ can also be written as

$$\rho = \sum_{k=1}^{K} p_k \,|\,\phi_k\rangle\,\langle\,\phi_k| \qquad \text{with} \qquad \sum_k p_k = 1, \tag{2.12}$$

where $K \in \mathbb{N}^+$ is *arbitrary* and the $|\phi_k\rangle$ are *arbitrary* unit vectors. In other words, the decomposition of ρ is, contrary to the classical case, non-unique, and ρ can now also be described as if it is behaving as an ensemble of systems of which a fraction p_k is in the state $|\phi_k\rangle$. We thus have diverse ensembles which are physically interpreted in a *completely different* way, but nevertheless are described by *the same* operator ρ, which according to the basic formalism of quantum mechanics (see postulate 1') is supposed to represent the physical state of the system. This would mean that physically different mixtures are assigned the same physical state.

This situation gives rise to two different positions. In the first position the two mixtures are considered to be *truly different*, even though the calculated expectation values for all measurable observables are the same. This implies that the state description through the operator ρ is *incomplete* and that the exact state preparation of the system is not taken into account. As such, this position is not forbidden by the set of quantum mechanical postulates. This position, taking the quantum mechanical state description being incomplete, is propagated by some famous physicists.

The second position is to hold that the quantum mechanical state description is *complete*, and that the different possible preparation procedures just do not show up in the state. This means that ρ in Eq.(2.12) doesn't characterize an ensemble of physical system *really being* in the states $|\phi_k\rangle$ with fractions p_k, but merely that an ensemble characterized through ρ acts upon measurement *as if* it is such an ensemble. In other words, the only thing quantum mechanics tells us is about measurement outcomes and not about the way in which the physical system is *in reality*, simply because there is nothing more to know, i.e. quantum mechanics is complete. This position is also taken in by some famous physicists.

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[5] In 1932 Von Neumann introduced the density operators ρ to create an ensemble theory for quantum mechanics. He introduced the extension of the Born postulate (postulate 3) for quantum mechanics to mixed states, and he suggested the measure $Tr[\rho P]$ (with P a projection operator). 25 years later Gleason's theorem showed that this measure is the only possible measure on the set of projection operators [47].

2.4.2 Interpretation of Mixed States; Composite Systems.

So far we have only considered single systems and the description of any composite systems was not taken into account. In treating *composite* systems, the same problem of interpreting mixed states becomes even more problematic. This will now be shown. Suppose a system $\mathcal{S}^{AB}$ is a system composed out of two subsystems $\mathcal{S}^A$ and $\mathcal{S}^B$. The Hilbert space of $\mathcal{S}^{AB}$ is given by the tensor product of the individual Hilbert spaces $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ (see appendix D for the theory of tensor products). Let ρ^{AB} be the state of $\mathcal{S}^{AB}$ and suppose that the systems have been separated and we perform a measurement on each of the subsystems alone. The observables of $\mathcal{S}^A$ are then represented by $A \otimes \mathbb{1}^B$ and the results of the measurement by operators of the form $P^A \otimes \mathbb{1}^B$. The corresponding probabilities are given by:

$$p_{\rho^{AB}}(P^A \otimes \mathbb{1}^B) = \mathrm{Tr}\,[(P^A \otimes \mathbb{1}^B)\rho^{AB}]. \tag{2.13}$$

Using the so-called partial trace we can define a density operator Tr^B on the Hilbert space $\mathcal{H}^A$ of S^A by means of:

$$\mathrm{Tr}^B[\rho^{AB}] := \sum_{j=1}^{N_B} \langle\, \phi_j |\, \rho \,|\, \phi_j \rangle \quad \in \mathcal{S}^A, \tag{2.14}$$

where $N_B = \dim\, \mathcal{H}_B$ and $\{|\, \phi_j\rangle\}$ is a set of eigenstates for $\mathcal{S}^B$. One readily computes that

$$\mathrm{Tr}\,[(P^A \otimes \mathbb{1}^B)\rho^{AB}] = \mathrm{Tr}[P^A \mathrm{Tr}^B[\rho^{AB}]]. \tag{2.15}$$

This means that for all measurements on $\mathcal{S}^A$ alone, the density operator Tr^B correctly gives the statistical properties of this system. Moreover, the same holds for $\mathcal{S}^B$ to which we can assign a density operator $\mathrm{Tr}^A\,[\rho^{AB}]$. In conclusion, the states of the subsystems A and B are the partial traces $\mathrm{Tr}^B\,[\rho^{AB}]$ and $\mathrm{Tr}^A\,[\rho^{AB}]$.

Now, the following results hold for the mixed state ρ of a composite system and its partial traces. For proofs see [47].

1. $\rho \in \mathcal{S}(\mathcal{H})$ of a composed system is in general not separable (i.e. cannot be written as $\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B$, with $p_i \in [0,1]$, $\sum_i p_i = 1$). The well-known bi-partite singlet states are an example of these non-separable states. .

2. If ρ is separable in the following way $\rho = \rho^A \otimes \rho^B$, then it is the case that the factors are equal to the partial traces, i.e.

$$\rho = \rho^A \otimes \rho^B \qquad \Longrightarrow \qquad \rho^A = \mathrm{Tr}^B\,\rho \quad \text{and} \quad \rho^B = \mathrm{Tr}^A\,\rho. \tag{2.16}$$

3. The partial traces determine ρ uniquely iff at least one of the partial traces is pure. In this case ρ is separable: $\rho = \rho^A \otimes \rho^B$.

4. The partial traces of ρ are pure iff ρ is pure and can be written as $\rho = |\,\phi\rangle \otimes |\,\psi\rangle\, \langle\,\phi| \otimes \langle\,\psi|$, where $|\,\phi\rangle \in \mathcal{H}_A$ and $|\,\psi\rangle \in \mathcal{H}_B$.

I will now show that from these results it follows that the interpretation of operators obtained by this procedure is *more problematic* than that of mixtures of the single system discussed in the previous section. In the latter case, upon giving up the completeness of the quantum mechanical state description, one could still interpret ρ as describing an ensemble of systems which *in reality* are in a certain state with specific relative fractions. However, for composite systems, this is no longer possible. That is, it is in general not possible to interpret the subsystem states ρ^A and ρ^B by means of a probability function over pure basis states $|\psi_i\rangle$, $|\phi_j\rangle$ representing the factual states of the subsystems. The proof follows by assuming it is possible and then showing a contradiction. Suppose this were possible, then ρ^A and ρ^B would describe mixtures

$$\rho^A = \sum_i q_i^A \,|\,\psi_i^A\rangle\,\langle\,\psi_i^A| \qquad \text{and} \qquad \rho^B = \sum_j q_j^B \,|\,\phi_j^B\rangle\,\langle\,\phi_j^B|\,, \tag{2.17}$$

and correlations would have to be contained in a joint probability q_{ij}^{AB} such that

$$\sum_j q_{ij}^{AB} = q_i^A, \quad \sum_i q_{ij}^{AB} = q_j^B. \tag{2.18}$$

For ρ^{AB} this means that it must be given by the following decomposition:

$$\rho^{AB} = \rho^A \otimes \rho^B = \sum_{i,j} q_{ij}^{AB} \,|\,\psi_i^A, \phi_j^B\rangle\,\langle\,\psi_i^A, \phi_j^B|\,. \tag{2.19}$$

However, this is in general not correct as can be seen from the following most general formulation of density operators for a bi-partite system:

$$\rho^{AB} = \sum_{i,j,k,l,m} p_m q_{ijm}^{AB} (q_{klm}^{AB})^* \,|\,\psi_i^A, \phi_j^B\rangle\,\langle\,\psi_k^A, \phi_l^B|\,, \tag{2.20}$$

with $\sum_m p_m = 1$, $0 \leq p_m \leq 1$ and $\sum_{ij} |q_{ijm}^{AB}|^2 = \sum_{kl} |q_{klm}^{AB}|^2 = 1$. Clearly the decomposition of Eq.(2.19) cannot be made equal to all possible density operators of Eq. (2.20).

In conclusion, we have seen that a general density operator ρ of the composed system can in general not be constructed from its partial traces. One could say that the system can not be separated into its subsystems. This is the so-called *principle of quantum inseparability* [55]:" If two systems interacted in the past it is in general not possible to assign a single state to either of the two subsystems." Thus even if we have a pure state of the composite system, the subsystems themselves can in general not be assigned any single state, i.e. these states are in general entangled. This study of the quantum mechanical state space of composite systems has shown us that *mixed states can not be identified with mixtures of states.* They are *not* just the classical statistical generalization of pure states to be able to treat unknown ensembles. Thus contrary to the classical case, maximal knowledge of the subsystems is in general not equivalent to maximal knowledge of the state of the total system. In other words, the state of the total system can in general not be determined from measurements on the subsystems.

These phenomena are all aspects of the so-called *quantum entanglement.* The next chapter is therefore completely devoted to this quantum entanglement.

2.5 Generalized Postulates of Orthodox Quantum Mechanics

Having discussed the extension of quantum mechanics to mixed states, we are now in the situation to state the generalized postulates [47]. These postulates together with the unchanged postulates 2 and 3 make up the so-called *orthodox* formalism of quantum mechanics.

1' *States (pure and mixed).* To every physical system corresponds a Hilbert space $\mathcal{H}$. Mixed states correspond bijectively with the density operators (or statistical operators) ρ in the interior of the convex set of states $\mathcal{S}(\mathcal{H})$, and the pure states correspond bijectively to the extreme elements, i.e. to density operators on the boundary $\partial\mathcal{S}(\mathcal{H})$ which are the one-dimensional projection operators. States of a bi-partite composed system correspond bijectively to states on the direct-product space of the subsystems Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, i.e. to elements of $\mathcal{S}(\mathcal{H}_1 \otimes \mathcal{H}_2)$.

2' *Observables-postulate.* To every physical quantity or observable $\mathcal{A}$ corresponds a self-adjoint operator A acting on $\mathcal{H}$.

3' *Spectrum-postulate.* The only possible outcomes of a measurement of observable $\mathcal{A}$ corresponding to the operator A are the values of the spectrum of A.

4' *Generalized Born rule (discrete case).* For a system in the state $\rho \in \mathcal{S}(\mathcal{H})$, upon measurement of A with a discrete spectrum (corresponding to the observable $\mathcal{A}$ with a finite set of possible outcomes), the probability for the measurement to yield a result a_i (an eigenvalue of A) is equal to

$$\mathrm{Prob}^{\rho}(a_i) = \mathrm{Tr}[P_{a_i}\rho] \tag{2.21}$$

where P_{a_i} projects onto the subspace spanned by all the eigenvectors of A corresponding to the eigenvalue a_i.

5' *Generalized Schrödinger-postulate.* The state of a system upon which no measurements are made during a certain time interval will evolve according to the unitary transformation

$$\rho(t) = U^{\dagger}(t - t_0)\rho(t')U(t - t_0), \tag{2.22}$$

with $U(t - t_0) = \exp[-iH(t - t_0)/\hbar]$ and with H the Hamiltonian of the system.

6' *Generalized Projection-postulate (discrete case).* If a measurement is performed on a physical system $\mathcal{S}$ in the state ρ of the operator A corresponding to the observable $\mathcal{A}$, and the result is the eigenvalue a_i of the spectrum of A, then the reduced state[6] directly after the measurement will be in the

[6] A much debated problem about these *state reductions* from ρ to ρ' is the fact that they cannot be the result of the Schrödinger evolution. This gives rise to the Measurement problem which is not dealt with here.

eigenspace corresponding to the eigenvalue a_i:

$$\rho \rightsquigarrow \rho' = \frac{P_{a_i}\rho P_{a_i}}{Tr\left[P_{a_i}\rho P_{a_i}\right]}. \tag{2.23}$$

Note that in the general case the P_{a_i} need not be one-dimensional.

2.6 Classification of Quantum States. Part I. Classification through the formalism

In this section I give a classification of the different states of a physical system as I have mentioned them in the previous sections, first for general systems (single or composite) and then for bi-partite composite systems. This classification has resulted naturally from the formalism of quantum mechanics and is therefore what I call a 'classification through the formalism'.

A: General Systems. Consider a system $\mathcal{S}$ with Hilbert space $\mathcal{H}$. The set $\{|\,\gamma_k\rangle\}$ forms an orthonormal basis for $\mathcal{H}$.

- **Pure states** correspond bijectively to (i) the extreme elements of the convex set $\mathcal{S}(\mathcal{H})$ of density operators, (ii) the one-dimensional projection operators of $\mathcal{P}(\mathcal{H})$, and (iii) the unit vectors in $\mathcal{H}$. That is, a pure state is represented as the vector state $|\,\psi\rangle$ and equivalently as the operator $\rho = P_{|\,\psi\rangle} = |\,\psi\rangle\,\langle\,\psi|$.
  - **Basis states** are states that are represented as a single basis vector in $\mathcal{H}$, e.g.. $|\,\psi\rangle = |\,\gamma_j\rangle$.
  - **Superposition states** are states that are represented as a superposition of basis vectors, e.g.. $|\,\psi\rangle = c_1\,|\,\gamma_1\rangle + c_2\,|\,\gamma_2\rangle$, where $c_1, c_2 \in \mathbb{C}$ and $|c_1|^2 + |c_2|^2 = 1$. These states are also called *coherent* superpositions.

  Note that the above definitions of a basis state and of a superposition state depend on the chosen basis.
- **Mixed states** are all non-pure states, i.e. they correspond to the density operators that are not extreme elements and can thus be decomposed into a convex combination of pure states. A mixed state is represented by $\rho = \sum_{i=1}^{N} p_i\rho_i$ with $\rho_i = |\,\gamma_i\rangle\,\langle\,\gamma_i| \in \mathcal{P}(\mathcal{H})$ and $i \in \mathbb{N}^+$. These states are sometimes called *incoherent* superpositions.

B: Composite Systems. Consider a bi-partite system $\mathcal{S}$ with Hilbert space $\mathcal{H}$ and which is composed out of two subsystems $\mathcal{S}_A$ and $\mathcal{S}_B$ with corresponding Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. The sets $\{|\,\alpha_i\rangle\}$ and $\{|\,\beta_j\rangle\}$ form an orthonormal basis for respectively $\mathcal{H}_A$ and $\mathcal{H}_B$.

- **Separable States** are states on the tensor product space $\mathcal{H}_A \otimes \mathcal{H}_B$ that can be written as $\rho = \sum_i p_i\rho_i^A \otimes \rho_i^B$, with $p_i \in [0,1]$, $\sum_i p_i = 1$

and where ρ_i^A and ρ_i^B are arbitrary states of the subsystems $\mathcal{S}_A$ and $\mathcal{S}_B$. The most simple separable states are $\rho = \rho^A \otimes \rho^B$, which are called *direct-product states.*[7]

- **Entangled states** are non-separable states, i.e. $\rho \neq \sum_i p_i \rho_i^A \otimes \rho_i^B$, with $p_i \in [0,1]$, $\sum_i p_i = 1$ and where ρ_i^A and ρ_i^B are arbitrary states of the subsystems $\mathcal{S}_A$ and $\mathcal{S}_B$. It is said that an entangled state has non-trivial correlations between the two subsystems that does not allow factorization. [8]

This classification of the different physical states in QM is mainly a result of the mathematical structure, i.e. of the tensor product characteristics of Hilbert spaces. In later chapters I will extend this classification by distinguishing many more different types of states when I consider more complex systems than the simple bi-partite systems.

2.7 The Orthodox and General Measurement Formalism

Quantum mechanics claims to be a universal theory and should thus be applicable to both microscopic systems such as atoms and macroscopic systems such as pointers of a measurement apparatus. However the microscopic systems are not directly observable. Consequently, in order to obtain any information at all about the microscopic system it is necessary to have it interact with a macroscopic system that can be directly observed. These interactions are usually called measurements [50].

I will take as the notion of a typical measurement the following situation: A quantum system $\mathcal{S}$ interacts with a measurement apparatus $\mathcal{M}$. This measurement apparatus has states that are assumed to be directly observable (pointer states). These pointer states ρ_P are affected by this interaction in a specific way depending on the states ρ_s of the system $\mathcal{S}$. In this way we can measure states ρ_s on $\mathcal{S}$ of the observable by observing pointer states ρ_P on $\mathcal{M}$. The specific way these pointer states are assumed to be correlated to the states of the system (i.e. the specific way the measurement is represented in terms of operators on the system $\mathcal{S}$), gives rise to two different types of measurement. These are the so-called *orthodox* and *general* measurements and are defined through two different sets of measurement postulates of the quantum formalism. These will be treated in the following two sections. The measurement postulates for the orthodox measurements have already been mentioned before, but will be reviewed for clarity and completeness.

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[7]It is in general very difficult to see whether or not a state is separable because no general algorithms exist. As we will see in section 3.1.1 only for very low dimensional tensor product Hilbert spaces necessary *and* sufficient conditions exist.

[8]See section 3.1.1 for a more formal definition of entanglement in arbitrary quantum states. And see also appendix D for a mathematical treatment of entanglement in bi-partite pure states in terms of the Schmidt decomposition. The issue of factorisability of correlations is treated in section 4.2.3.

2.7.1 Orthodox Measurements

Following Von Neumann, I will now assume that pointer positions of the measuring apparatus $\mathcal{M}$ after the measurement interaction map *uniquely* onto eigenvalues of the system $\mathcal{S}$[9]. Because of this one-to-one correspondence of pointer states to eigenvalues one can thus consider the system itself, without further reference to the measurement apparatus. Further, it is assumed that for this measurement situation the earlier mentioned measurement postulates of the orthodox formalism of QM hold (i.e. the Observables-postulate (2), the Spectrum-postulate (3), the generalised Born-rule (4') and the generalised Projection-postulate (6')).

Let According to these postulates every observable is represented by a self-adjoint operator. Every self-adjoint operator A has from the spectral theorem a unique spectral resolution in terms of the eigenvalues a_i and the eigenprojections P_{a_i}: $A = \sum_i a_i P_{a_i}$. The eigenprojections satisfy

$$\sum_i P_{a_i} = \mathbb{1} \quad , \quad P_{a_i} P_{a_j} = \delta_{ij} P_{a_i}. \tag{2.24}$$

The set of orthogonal projections $\{P_{a_1}, \ldots , P_{a_n}\}$ that satisfy Eq.(2.24) is called a *spectral resolution* [94]. Furthermore, from the measurement postulates in the orthodox formalism it follows that the probability $p(a_i)$ that the result a_i is obtained upon measurement is given by $p(a_i) = Tr[\rho P_{a_i}]$ and the state ρ' immediately after the measurement is given by the 'collapse' $\rho \rightsquigarrow \rho' = \frac{P_{a_i} \rho P_{a_i}}{Tr[P_{a_i} \rho P_{a_i}]}$. This type of probability measure, which uses the spectral resolution of the identity in orthogonal projection operators, is referred to as a projection valued measure (PV measure), i.e. each outcome has a probability determined by a measure in terms of orthogonal eigenprojectors (e.g. P_{a_i}). These measurements are also called *Von Neumann* measurements, *projective* measurements or *ideal* measurement.

This orthodox measurement formalism has an alternative but equivalent formulation [94] where one starts from the postulate that every observable is represented by a mapping

$$\mathcal{A} : a_i \rightarrow P_{a_i} \tag{2.25}$$

from a set $\{a_1, \ldots , a_n\}$ of real values to a spectral resolution. The spectral theorem tells us that these mappings are in one-to-one correspondence to self-adjoint operators A. In this formalism the observable corresponds to a spectral resolution on the space of eigenvectors that correspond to the eigenvalues of the observable. In this alternative approach a specific spectral resolution of the identity is taken to be the starting point and not the self-adjoint operators. It is this second approach which allows generalization to the formalism of general measurements.

The underlying assumption of the orthodox measurement procedure is that the measurement is *repeatable* for subsequent identical measurements. Measuring directly after the first measurement the same observable again, will always lead to the same outcome. This follows from the projection postulate and the fact that $P_{a_i} P_{a_i} = P_{a_i}$.

In practical situations this repeatability is not always the case, and we have to extend the formal representation of measurement to deal with these non-ideal

[9]This assumption is non-trivial, but one is able to write down specific interactions such that this is possible [50].

cases. This is one of the motivations for the extension of the orthodox formalism to the formalism that includes general measurements. A further motivation for this extension is that not all measurement procedures can be described using the orthodox formalism. Let me now introduce this extended formalism.

2.7.2 General Measurements and the Extended Quantum Formalism

The extension of the set of quantum mechanical measurements to include more general measurements can be done in several ways. Here I will take the view that an extension of the formalism of QM itself is needed for this purpose[10]. A more liberal set of measurement postulates will thus be presented.

The key difference between the formulation of the general measurements and the orthodox measurements is the replacement of the usage of the spectral resolution by the usage of a semi-spectral resolution [94]. Such a semi-spectral resolution is defined as a set of positive operators $\{E_1, \ldots, E_n\}$ on $\mathcal{H}$ that give the following partition of unity:

$$E_i \geq 0 \ , \qquad \sum_i E_i = \mathbb{1}. \tag{2.26}$$

Note that the operators E_i need not be projection operators.

Using this semi-spectral resolution a POV measure (POVM) can be defined as follows [44]. A POV measure is a set function E which maps measurable subsets $\Delta \in \mathbb{R}$ to positive operators $E(\Delta)$ comprising a semi-spectral resolution such that for any state ρ:

$$\Delta \mapsto \mu_E^\rho(\Delta) := \mathrm{Tr}[\rho E(\Delta)] \tag{2.27}$$

is an ordinary probability measure on $\mathbb{R}$, i.e. $E(\mathbb{R}) = \mathbb{1}$ and for any sequence of disjoint measureable sets $\Delta_i \in \mathbb{R}$,

$$E(\cup_i \Delta_i) = \sum_i E(\Delta_i). \tag{2.28}$$

Here $\mu_E^\rho(\Delta)$ is the probability in the state ρ for the outcome of the measurement with the POVM to be in Δ. In order to describe the measurement using a POVM the so-called operations R_δ are needed. These are a family of linear operators decribing the change of the quantum state during the measurement. If the outcome $\delta \in \mathbb{R}$ is obtained then the state is affected in the following way:

$$\rho \rightsquigarrow \rho' = \frac{R_\delta \rho R_\delta^\dagger}{\mathrm{Tr}[R_\delta \rho R_\delta^\dagger]}. \tag{2.29}$$

The operations R_δ determine the POV measure E as follows:

$$E(\Delta) = \sum_{\delta \in \Delta} R_\delta^\dagger R_\delta. \tag{2.30}$$

[10] However, not everybody agrees with this extension of the formalism. Some authors want to hold on to the orthodox formalism and present the general measurements not as fundamentally different requiring new postulates but as arising from certain orthodox measurements on a larger system. See also footnote 6.

Note that POV measures include as a special case the PV measures where all positive operators are orthogonal projection operators. In an orthodox measurement of a PVM the operations R_δ are equal to the projection operators $P_\delta = E(\delta) := E(\{\delta\})$. This gives the usual projection postulate. Further note that in general there are *many* classes of possible operations R_δ giving rise to the same POV measure via $M(\delta) = R_\delta^\dagger R_\delta$.

Having presented POV measures, the postulates for the quantum formalism that incorporates generalized measurements are as follows (postulates 1' and 5' remain unchanged):

1" *States (pure and mixed).* To every physical system corresponds a Hilbert space $\mathcal{H}$. Mixed states correspond bijectively with the density operators (or statistical operators) ρ in the interior of the convex set of states $\mathcal{S}(\mathcal{H})$, and the pure states correspond bijectively to the extreme elements, i.e. to density operators on the boundary $\partial\mathcal{S}(\mathcal{H})$ which are the one-dimensional projection operators. States of a bi-partite composed system correspond bijectively to states on the direct-product space of the subsystems Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, i.e. to elements of $\mathcal{S}(\mathcal{H}_1 \otimes \mathcal{H}_2)$.

2" *Observables (general measurements).* An observable is postulated to be represented by a mapping $\mathcal{E} : e_i \to E_i$ from a spectrum $\{e_1, \dots, e_n\}$ to a semi-spectral resolution. The positive operators E_i are elements of the POV measure E with $E_i := E(e_i)$ for e_i in the spectrum. The spectrum is identical to the set of possible values. Using Uffink's words [94], note that because there is no such theorem as a 'semi-spectral theorem' it is impossible to uniquely characterize the general observables by self-adjoint observables.

3" *Spectrum-postulate (general measurements).* The set of all possible results that can be obtained in a measurement of an observable is determined by the measurement setup and composed out of a spectrum $\{e_1, \dots, e_n\}$ which needs not be necessarily composed out of real numbers.

4" *Born rule (general measurements).* The probability of obtaining the value e_i in a measurement of observable $\mathcal{E}$ on a system in the state ρ is given by

$$Prob^\rho(e_i) = \mathrm{Tr}[\rho E_i] = \mathrm{Tr}[R_i \rho R_i^\dagger], \tag{2.31}$$

where $\mathrm{Tr}[\rho E_i] \geq 0$ and $\sum_i \mathrm{Tr}[\rho E_i] = 1$. Here E_i is a positive operator of the semi-spectral resolution (non-uniquely) determined by $R_i R_i^\dagger$. This probability measure is the positive operator valued measure (POVM) corresponding to the observable.

5" *Generalized Schrödinger-postulate.* The state of a system upon which no measurements are made during a certain time interval will evolve according to the unitary transformation

$$\rho(t) = U^\dagger(t - t_0)\rho(t')U(t - t_0). \tag{2.32}$$

with $U(t - t_0) = \exp[-iH(t - t_0)/\hbar]$, with H the Hamiltonian of the system.

6" *Projection-postulate (general measurements).* If a general measurement of observable $\mathcal{E}$ is performed on a physical system $\mathcal{S}$ in the state ρ and the result is the value e_i, then the state directly after the measurement will be given by the 'collapse'

$$\rho \rightsquigarrow \rho' = \frac{R_i \rho R_i^\dagger}{\mathrm{Tr}[R_i \rho R_i^\dagger]}. \tag{2.33}$$

This generalized measurement formalism using a semi-spectral resolution and POVMs leads to new types of observables for general types of measurements such as special types of non-ideal measurements and collective or sequential measurements. These will be used in chapters 5 and 6.

As an example I will treat a non-ideal measurement where due to imperfections of the measurement apparatus $\mathcal{M}$ there might be a whole family of states ρ_k of the system $\mathcal{S}$ each of which, with some probability $\lambda_k > 0$, give rise to the observed measurement outcome e_i (the pointer position corresponding to this value). Instead of a single projection operator on a single state (such as $P_{e_i} = |\,\psi_i\rangle\,\langle\,\psi_i|$) to represent these non-ideal but more realistic measurements, we should use a weighted measure over the set of projection operators on the state space of the system $\mathcal{S}$. This is the extension to the positive operator valued measure E_i:

$$E_i = \sum_k \lambda_k^i\,|\,\psi_k\rangle\,\langle\,\psi_k|\,, \tag{2.34}$$

with $\sum_i E_i = \mathbb{1}$ and $\{\,|\,\psi_k\rangle\,\}$ orthonormal and complete. Using the collection of these operators E_i which make up a POVM, the non-ideal measurements on the system can be adequately represented. The probability to obtain a result e_i is then not given by $\mathrm{Tr}[\rho P_{e_i}]$ using a single projection operator but by $\mathrm{Tr}[\rho E_i] = \sum_k \lambda_k^i$ $\mathrm{Tr}[\rho\,|\,\psi_k\rangle\,\langle\,\psi_k|]$. The distribution of the variable λ_k^i determines the 'sharpness' of the measurement. E.g. for $\sum_k \lambda_k^i = \delta_{ik}$ the measurement is at its 'sharpest' since it reduces to an ideal projective measurement.

Orthodox measurements are a special case of general measurements (in case that the positive operators are projection operators). As the earlier given example of a non-ideal measurement has pointed out, one could say that in fact all real measurements are general measurements in terms of POVMs and that to a very good approximation they might be orthodox measurements using PVM's. However, it can be shown that any POVM can be realised by performing a PVM on a larger system. This is Neumark's theorem [50].

The orthodox measurement formalism where operators are represented by self-adjoint operators is by far the most popular although awareness of the general measurements and their POVM representation is slowly growing. Because of this reason the orthodox measurement formalism will be used in this treatise as the standard formalism. Only when explicitly mentioned otherwise (e.g. in chapter 6) I will use the formalism using general measurements.

2.8 Measurement Compatibility

The question of whether two or more physical quantities are *compatible* is often regarded synonymous with the requirement that these quantities can be measured *simultaneously.* In classical physics all observables are considered to be compatible, but in quantum theory the situation is different. As a direct consequence of the quantum formalism, many pairs of observables are not simultaneously measurable, i.e. are incompatible, because of non-commuting operators Of course this statement requires a clear definition of what is meant by 'a simultaneous measurement'. I will pursue this question in section 2.8.2. First I will focus on the standard account of the idea of measurement compatibility in quantum mechanics.

2.8.1 Standard Account of Measurement Compatibility in Quantum Mechanics

As a first requirement we need the following important theorem:

Theorem 2.8.1. *If two self adjoint operators A and B commute, then there exists a maximal self-adjoint operator C of which A and B are functions, i.e. $A = f(C)$ and $B = g(C)$.*[11] *(For proof see Redhead [46], page 18.)*

Notice that if we can write $A = f(C)$ for an observable A as a function of some maximal observable C, then the choice of C is by no means unique. If the map f is not 1:1, then there will always exist another maximal operator C' such that $A = g(C')$, and C and C' do not commute, $[C, C'] \neq 0$. They do commute iff A itself is maximal. Since in this case f can be inverted: $C = f^{-1}(A) = f^{-1}(g(A))$, from which it follows that $[C, C'] = 0$.

In the standard account the idea of compatibility of observables can now be formulated in terms of the functional relationships between these observables, i.e. two observables A and B are said to be *trivially compatible* [45] if there is a third observable C and functions $\mathcal{F}$ and $\mathcal{G}$ such that $A = \mathcal{F}(C)$ and $B = \mathcal{G}(C)$. Thus a number can be ascribed to both A and B by a single measurement of C. Now theorem (2.8.1) implies that if A and B are trivially compatible they must commute, and because A and B are normal operators the converse follows as well. In other words, we can state that observables A and B can be said to be trivially compatible iff the operators that represent them commute with each other. More generally speaking this applies to any set of self-adjoint operators $\{A_1, A_2, \ldots, A_k\}$ that commute in pairs. However, there are many pairs of self-adjoint operators that do not commute and hence many sets of observables that are not trivially compatible. The question then arises if there are any pairs of observables that are of this type (i.e. they are not trivially compatible) but still are compatible in the sense that they can be measured simultaneously in some way. Clearly this depends on what is meant by 'measured simultaneously'.

Von Neumann [19] has given a detailed account of what it means for two observables to be simultaneously measurable and he concluded[12] that "The commutativity of operators A and B is necessary and sufficient for the simultaneous measurability of [observables] $\mathfrak{A}$ $\mathfrak{B}$. Ref. [19], p. 228. In other words, according to Von Neumann, the only observables that are simultaneously measurable (compatible) are observables that are trivially compatible. He thus identified

[11] See Appendix C, Eq.(C.8) for the definition of a function of an observable.

[12] See Isham [45], page 100, for a detailed analysis of von Neumann's assumptions leading to this conclusion.

compatibility with commutativity and this has become a widely used practise in quantum mechanics.

2.8.2 Critique of Standard Account

With this last identification we arrive at the starting point for my critique of the standard account of measurement compatibility and of simultaneous measurement in quantum mechanics.

First a short semantical note. The question of simultaneous measurement has not so much to do with the temporal issue of measurement *at the same time* but rather has to deal with the issue of *non-conflicting measurement setups*, i.e. of whether one and the same measurement setup can allow for measurement of all observables involved. Thus observables which are not simultaneously measurable do not allow to be measured using non-conflicting measurement setups and as a consequence cannot be measured at the same time (on the same system). Having this is in mind, simultaneous measurement and measurement compatibility thus actually means *measurement setup compatibility*: two observables are compatible iff they allow for non-conflicting measurement setups.

Now let me go back to the standard account of measurement compatibility of observables in quantum mechanics. As we have seen all mutually commutative operators are considered to be compatible (i.e. they are called trivially compatible) and further according to Von Neumann these are *all* considered to be compatible. In other words, commutativity implies compatibility and if we follow von Neumann the converse is supposed to be true as well.

However, I question this account of compatibility because, following Harvey Brown [83], "the root issue is not mathematical commutativity but measurement compatibility, and the former is certainly not a sufficient condition for the latter." The only thing quantum mechanics tell us is that measurement compatibility implies commutativity, not the other way around. The identification of measurement compatibility with commutativity is to overlook the deeply rooted physical aspect of it and to jump too easily to the safe ground of mathematics[13]. To see this look at the following example first presented in different form by Harvey Brown. Suppose one wants to measure on a bi-partite spin-$\frac{1}{2}$ system, where each of the subsystems is spatially separated, the operators A and B where $A = \sigma_x \otimes \sigma_z$ and $B = \sigma_z \otimes \sigma_x$. According to the standard account these two measurements are simultaneously measurable (compatible) because A and B commute. However, how does one measure each of the two operators? Because of the spatial separation of the two particles a natural way to measure operator A is to measure σ_x and σ_z separately on each of the two particles and then take the product of their results. However if the same procedure is used to measure operator B then this amounts to measuring the non-commutative operators σ_x and σ_z on each of the two particles, which is clearly not possible. Then, what other measurement procedures can be envisaged that would allow for measurement of the commuting A and B? Perhaps some sort of holistic non-local measurement that is as yet unknown how to perform? To cut this question short, it seems that although

[13] Another example of this misunderstanding of what measurement compatibility means will be found in section 4.3.3 where I argue that certain Bell-theorems cannot be experimentally implemented because of the usage of sets of commuting but nevertheless incompatible observables.

we are dealing with mutually commutative operators they seem to be nevertheless not measurement compatible because no measurement setup is available for simultaneously measuring the operators.

This example shows us that the trivialness of the so-called trivial compatible observables in the standard account raises serious doubt. And further, the inference by von Neumann that all commutative observables are compatible (i.e. can be measured simultaneously) is seen to be questionable.

2.8.3 Complete Sets of Commuting Observables

I will not elaborate any further on the question of simultaneous measurability, but instead go back to the sets of trivially compatible observables, i.e. sets of pairwise mutually commuting operators $\{A_1, A_2, \ldots, A_k\}$. It is easy to see that if two operators commute, it is always possible to find a basis relative to which they are simultaneously diagonal, and thus both operators then have all eigenvectors in common. Now, suppose we look for a *maximal* set of commuting observables, that is we cannot add any more observables to our list without violating the pairwise commutation requirement. Then the following theorem holds:

Theorem 2.8.2 (Complete Set of Commuting Observables (CSCO)). *On any finite Hilbert space $\mathcal{H}$ there are finite sets of self-adjoint operators that commute in pairs and whose simultaneous eigenvectors form a basis set for $\mathcal{H}$ with no residual degeneracy. These are the maximal sets of trivially compatible observables. (For proof see [45]). Any sets with residual degeneracy can be made into one of these non-degenerate sets by the addition of a finite set of pair-wise commuting operators.*

In other words the set of eigenstates of a CSCO is a basis for $\mathcal{H}$. In general there are many of such different CSCOs[14], and any pure state is a joint eigenstate of a certain CSCO.

Now suppose we have two different CSCOs, each of them providing a basis of joint eigenstates. Because these sets are different not all operators mutually commute in pairs, which implies that not all eigenstates of each set are eigenstates of the other set. No complete state description exists that is an eigenstate for *all* possible observables which can be measured on the system. In other words, no physical states exists that attribute well defined values (i.e. eigenvalues) to all possible observables. This fact is the basis of the *indeterminacy relations*[15]:

2.8.4 Joint Probabilities

For many applications of quantum mechanics one wants to be able to compute *joint probabilities* for compatible observables to yield certain outcomes. From the-

[14] As a well known example of the non-uniqueness of the CSCO consider two particles, labeled 1 and 2, each with a total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$ (spin $\mathbf{S}$ and orbital angular momentum $\mathbf{L}$). There are two different maximal sets of trivially compatible observables, each providing a complete but different set of basis states. Firstly, the simultaneous eigenstates of $\mathbf{J_1^2}$, $\mathbf{J_2^2}$, J_{1z}, and J_{2z} denoted by $|\, j_1 j_2; m_1, m_2\rangle$, and secondly the simultaneous eigenstates of $\mathbf{J^2}$, $\mathbf{J_1^2}$, $\mathbf{J_2^2}$ and J_z denoted by $|\, j_1 j_2; jm\rangle$. These two basis sets are connected by a unitary transformation whose matrix elements are called the Glebsch-Gordon coefficients.

[15] Also called the *uncertainty relations*.

orem 2.8.2 it follows that any vector $|\psi\rangle \in \mathcal{H}$ can be expanded in terms of the associated simultaneous eigenvectors $|a_{1i_1}, a_{2i_2}, \ldots, a_{ki_k}\rangle$ (with $A_k\,|a_{1i_1}, a_{2i_2}, \ldots, a_{ki_k}\rangle = a_{ki_k}\,|a_{1i_1}, a_{2i_2}, \ldots, a_{ki_k}\rangle$) as :

$$|\psi\rangle = \sum_{i_1,i_2,\ldots,i_k} c_{i_1,i_2,\ldots,i_k}\,|a_{1i_1}, a_{2i_2}, \ldots, a_{ki_k}\rangle\,, \tag{2.35}$$

with $c_{i_1,i_2,\ldots,i_k} = \langle a_{1i_1}, a_{2i_2} \ldots, a_{ki_k}|\psi\rangle$ and where the sum in Eq.(2.35) is over the eigenvalues of the operators $\{A_1, A_2, \ldots, A_k\}$.

The basic probabilistic rule of Postulate 4' now becomes the statement that if the state vector is $|\psi\rangle$, and if a simultaneous measurement is made of the trivially compatible observables $\{A_1, A_2, \ldots, A_k\}$ the *joint probability* that the results obtained will be $a_{1i_1}, a_{2i_2}, \ldots, a_{ki_k}$ is

$$\mathrm{Prob}^{|\psi\rangle}(A_1 = a_{1i_1}, A_2 = a_{2i_2}, \ldots, A_k = a_{k,i_k}) = |\langle a_{1i_1}, a_{2i_2}, \ldots, a_{ki_k}|\psi\rangle|^2 . \tag{2.36}$$

(An extension to include mixed states using the density operators ρ is obvious.)

2.9 Conclusion and Summary

In this chapter the basic mathematical structure of quantum mechanics has been presented. Three different sets of postulates were obtained. They resulted from two generalizations of the set of postulates for pure states and projective measurements. The first was the generalization of pure states to mixed states. This completed the structure of orthodox quantum mechanics. The second generalization was the extension from projective measurements to general measurements. This is the extension of projection valued measures (PVM) to positive operator valued measures (POVM). This resulted in the set of postulates of quantum mechanics for general measurements. Extending the formalism has resulted in a classification of the quantum state space into different states.. This classification will be extended in the following chapters.

Because quantum mechanics primarily deals with measurement outcomes it became necessary to give the standard formulation of measurement compatibility (i.e. simultaneous measurability) of observables. We have seen that in the standard account measurement compatibility was identified with commutativity. I have criticized this identification and have argued that commutativity is not sufficient for measurement compatibility.

Chapter 3

Entanglement: Separability, Distillability and Quantum Information.

In this chapter I will consider quantum entanglement and various issues connected to it[1]. In section 3.1 I will present the idea of entanglement in a very general context, namely as the phenomenon of quantum inseparability. This is formalised through the definition of an entangled state as a non-separable state. Therefore the separability properties of density operators are discussed. This leads to a classification given in section 3.2 of bi-partite, tri-partite and N-partite entangled systems. In the next section, section 3.3, the family of entangled states (pure and mixed) are investigated to see whether or not they can be distilled or purified to specific pure states (i.e. the maximally entangled states). This allows for an investigation in section 3.3.1 of the relationship between the distillability and separability properties of bi-partite density operators. Lastly, the classification of different quantum states, given in the previous chapter, will be extended by a second classification through entanglement properties and aspects of quantum information.

3.1 Introduction to Entanglement

It is the year 1935 and the beginning of a particular branch of quantum theory, namely the theory of entanglement. In this year both the famous paper of Einstein, Podolsky and Rosen [56] (EPR) and, in a reaction to the EPR paper, Schrödinger's article [57] in which he first mentioned the term "verschränkter Zustand" (entangled state) appeared. Although providing major contributions, both Einstein and Schrödinger were expressing deep dissatisfaction with the development of quantum theory and were especially struggling with one of the most striking features of the quantum formalism, i.e. with *entanglement*. This entanglement or also called *the principle of quantum inseparability* [55] can be expressed for pure states as follows: *"If two systems interacted in the past it is in general not possible to assign a single state vector to either of the two subsystems."* If this is the case, the state of the composite system is entangled. This is contrary

[1]The structure of this chapter has benefited much from Ref. [59].

to the classical case[2] where each subsystem in a composite system can always be assigned a single physical state. In order to extend the idea of entanglement to general quantum states, a sharp mathematical definition of entanglement for composite states is needed. The mathematical characterization was given by Werner in 1989 [65]. I restrict myself here to the most simple composite systems: bi-partite systems of finite dimension for which Werner has given the following *extended* principle of quantum inseparability: *" If two systems interacted in the past it is possible to find the whole system in the state that cannot be written as a mixture of product states"*. This principle leads to the following definition of general (pure and mixed) entangled states.

Definition 3.1.1. *A state ρ is* entangled *or* inseparable *iff it cannot be written as a convex combination of direct-product states:*

$$\rho^{AB} \neq \sum_i p_i \ \rho_i^A \otimes \rho_i^B \tag{3.1}$$

with $\sum_i p_i = 1$.

Conversely, bi-partite states which do allow a decomposition in terms of a convex combination of product states are *separable*. The most simple examples of separable states are the direct-product states, i.e. $\rho = \rho^A \otimes \rho^B$. The convex hull of such direct-product states is the set of separable states.

Note that one could thus say that because of the above definition the question of entanglement has been reduced to the mathematical problem of inseparability of a quantum state. But things are not all this clear when considering the consequence of the specific correlations inherent in entangled quantum states. This is first addressed by the criticism of the EPR paper of 1935. The EPR criticism that quantum mechanics was incomplete using their criterium of local realism, had provoked many reactions. John Bell proved [60] that local realism implies constraints on the predictions of spin correlations in the form of inequalities (the so-called Bell-inequalities) which can be violated by quantum-mechanical predictions for entangled quantum states. Consequently it is said that quantum mechanics has non-classical correlations. This latter feature of quantum mechanics is one of the most striking features of entanglement. The Bell-inequalities require correlations between the outcomes of measurements performed on separated systems which have interacted in the past. This feature of 'non-classicality' emphasizes the specific correlation aspect of entanglement.

Quantum mechanics allows thus for correlations between subsystems that are classically not possible. Entanglement has therefore been a major example of the feature of *quantum correlations as opposed to typical classical correlations.* The specific relations between features of quantum states and the so-called local and classical correlations will be treated in chapter 4 where we will see that the specific way the state space of quantum mechanics is tied to the classical structure is highly non-trivial.

[2] See appendix F for the difference between the classical and quantum mechanical state space.

3.1.1 The Separability Problem

Above I have defined entangled states and have distinguished two aspects of entanglement. However for greater understanding I will present the feature of entanglement in some historical context. Suppose we have a state ρ of a composite system with state space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Perhaps surprisingly, but the question whether or not this state is entangled will in general be hard to answer [59].

Up until about 1989 the answer seemed to be rather straightforward: a quantum system is entangled if the observables of the different subsystems are correlated in such a way that their measurement outcomes will be 'non-local' in the sense that they show violation of a Bell-inequality. Indeed, for bi-partite pure states it is enough to check if no local hidden variable model can account for the correlations between the observables in each subsystem to show entanglement: violating a Bell-inequality is a sufficient and necessary criterium for bi-partite entanglement (see section 5.2.1). Entangled states were therefore for a long time defined as those states that violate a Bell-inequality.

However, nowadays it is known that this is not all the case when dealing with mixed states or more complex systems. Let me give an example of this using mixed bi-partite states. As will be shown, the separable bi-partite states can all be modeled by a local hidden variable theory and thus satisfy Bell's inequalities. However, Werner showed that the converse is not true; he exhibited an important class of mixed states, now known as the 'Werner states' which *do* posses a local hidden variable model for any projective measurements and thus satisfy the Bell-inequality, but which are nevertheless *not* separable.

Subsequently, examples of states, including certain Werner states, were found which did not violate any Bell inequality for usual projective measurements, but which would show violation if subjected to a sequence of local measurements or to local collective operations. This feature is the so called 'hidden entanglement' [52], which will be extensively treated in chapter 5.

This hidden entanglement has raised the question, which has remained open, whether any inseparable state would violate some generalized Bell-inequality. As a consequence, the equivalence for pure bi-partite states between entanglement and violation of a Bell inequality is found to be no longer adequate for mixed states. Thus contrary to pure states, mixed states show a much richer and complex structure in their state space and the full set of quantum correlations they can exhibit is still not fully known. Because of this and because of the difficulties associated with producing Bell-inequalities or defining local hidden variable models for particular mixed states, an entangled state was subsequently defined as one which was not separable. This is the definition used above. Under this approach attention thus moved from probability distributions arising from measurements on the state to the form of the state itself. General conditions for separability were sought and this turned out not to be an easy task. This is the content of the separability problem: *Given a composite system in the state ρ, is it separable or not?*

3.1.2 Partial Transpose Criterium

The separability problem is mainly a technical problem about the testability and implementability of the definition of separability. A first step towards answering this technical problem is the necessary condition for separability derived by Peres in 1996 and further elaborated on by the Horodecki's. Peres [61] provided a powerful necessary condition for separability of all mixed states, and the Horodecki's [62] showed that this is also a sufficient condition for composite Hilbert spaces of dimension 2×2 and 2×3. These conditions use the partial transposition of a density matrix ρ (see appendix E for a formal definition).

First let me define the transpose $\mathcal{T}$ of an operator N in terms of the matrix elements with respect to a given basis $\{|\, i\rangle\}$:

$$\mathcal{T} : N \longrightarrow N^T \equiv TN \quad \text{with} \quad \langle\, k|\, N\,|\, l\rangle = \langle\, l|\, N^T\,|\, k\rangle\,. \tag{3.2}$$

As shown in appendix E this is a trace-preserving positive, but not completely positive map. Thus the extension to the *partial transpose* $\mathcal{PT} \equiv T_A \otimes \mathbb{1}_B$ is not positive on the composite system. This partial transpose $\mathcal{PT}$ of an operator O on $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ with respect to the first subsystem is given by $O^{T_A} \equiv T_A \otimes \mathbb{1}_B O$ and is defined in terms of is matrix elements with respect to a given basis $\{|\, i, j\rangle\}$ by:

$$\mathcal{PT} : O \longrightarrow O^{T_A} \equiv T_A \otimes \mathbb{1}_B \quad \text{with} \quad \langle\, kl|\, O\,|\, mn\rangle = \langle\, ml|\, O^{T_A}\,|\, kn\rangle\,. \tag{3.3}$$

Note that O^{T_A} is basis-dependent but its spectrum (i.e. its set of eigenvalues) is not. A self adjoint operator O has positive partial transposition (PPT) iff all the eigenvalues of O^{T_A} (and all other partial transpositions) are non-negative , i.e. a density operator ρ is said to be a *PPT state* iff all partial transpositions are positive. On the other hand, an operator has non-positive partial transposition (NPPT) iff at least one eigenvalue of a partial transposition is negative. NPPT is also called 'negative partial transposition' (NPT).

In order to present the partial transpose criterium, recall that a density operator ρ of two systems A+B is separable iff it can be written as

$$\rho = \sum_i p_i \rho_i^{(A)} \otimes \rho_i^{(B)}, \tag{3.4}$$

with $p_k > 0$ and $\sum_i p_i = 1$.

Under the partial transpose $\mathcal{PT}$ it follows that the separable density operator of Eq.(3.4) transforms as follows:

$$\rho \longrightarrow \rho^{T_A} = \sum_i p_i \left(\rho_i^{(A)}\right)^T \otimes \rho_i^{(B)}. \tag{3.5}$$

From appendix E we know that because T is positive $\left(\rho_i^{(A)}\right)^T$ is again a density operator. Therefore ρ^{T_A} is again a density operator. We now look at the eigenvalues of ρ^{T_A}. If ρ is separable then ρ^{T_A} has positive eigenvalues. Therefore, if ρ^{T_A} has one or more negative eigenvalues, the original density operator ρ must have been non-separable, i.e. entangled. The same holds for the case of ρ^{T_B}

This is the partial transposition criterium for separability and can now be expressed in the following two theorems [59]:

Theorem 3.1.1. *If ρ is separable then all partial transpositions are positive, i.e.* $\rho^{T_A} \geq 0,\ \rho^{T_B}$

Thus, being a PPT state is a necessary condition for separability.

Theorem 3.1.2. *If* $\rho^{T_A} \geq 0,\ \rho^{T_B} \geq 0$ *for spaces of dimensions* 2×2 *and* 2×3*, then ρ is separable.*

In general there exist PPT states that are not separable (and thus entangled) in $M \times N$ spaces with $M = 2, N \geq 4$ or $M, N \geq 3$. These PPT entangled states have been termed 'bound entangled states' to distinguish them from 'free entangled states'. These names are associated with distillability properties that will be discussed in section 3.3. 'Bound entangled states' are entangled, but as we shall see in the next chapter no matter how many copies used, it is impossible to 'distill' them via local operations and classical communication (LOCC) to the form of a maximally entangled state. New questions thus arise: *What distinguishes separable states from PPT states? Are all NPPT states (NPT states) distillable (i.e. 'free entangled')?* These questions will be elaborated on after the introduction of the distillability problem in section 3.3.

3.1.3 Quest for Separability Criteria

Let's go back to the partial transposition criterium of theorems 3.1.1 and 3.1.2. As we have seen, transposition of a density matrix is an example of a positive map. This is not a coincidence; the problem of separability in higher dimensions is approached by looking for positive maps which result in a negative operator and hence reveal the entanglement. A general sufficient condition for separability has been found:

Theorem 3.1.3. *If for all positive maps Λ, the state* $(\Lambda^A \otimes \mathbb{1}^B)\rho^{AB}$ *is always positive, then* ρ^{AB} *is separable [62].*

However, note that the application of this theorem needs a classification of all positive maps and this is as yet unsolved.

Another approach to the separability problem is in terms of the search for the so-called *entanglement witnesses*. These are certain observables E which are supposed to reveal the entanglement of an entangled state. The search for such witnesses is guided by the following theorem.

Theorem 3.1.4. *If ρ is entangled then there exists an entanglement witness E such that* $Tr[E\rho_{sep}] \geq 0$ *and* $Tr[E\rho] < 0$ *for all separable operators* ρ_{sep} *[59].*

Entanglement witnesses represent in some sense a kind of Bell inequality which is violated by the entangled state ρ. The construction of the witnesses E is a difficult problem and still under investigation [59].

The quest for sufficient and necessary separability criteria is still going strong, i.e. new results appear every month, but these will here not be further elaborated on. Rather I will present in the next section an interpretation of separability from a physical point of view.

3.1.4 Physical Interpretation of Separability.

In this section I will try to interpret the principle of separability from a 'physical point of view'. It uses the (intuitive) idea that local operations and classical communication cannot produce any non-classical effects such as entanglement. In other words, two parties A and B, each starting with any particular state ρ^A and ρ^B can try to locally operate and correlate these states, but they will only be able to produce separable states $\rho^{AB} = \sum_i p_i \; \rho_i^A \otimes \rho_i^B$. Before trying to explain this intuitive idea we have to know what is meant by local operations and classical communication (LOCC)[3]. This will now be presented:

1. Local operations
   - *Local transformations and measurements.* These are any completely positive linear and trace-preserving map of the density operator of the first party that leaves unchanged the state of the second party. Such transformations need not be unitary and can in general be modeled by local positive maps, i.e maps acting on only one subsystem. Examples are rotations, local permutations, etc.
   - *Selective local operations.* Depending on the outcome of local measurements (and classical communication) each party can select a subset from their ensemble of states. An example of this is post-selection, i.e. two parties A and B can perform non-trace preserving selective operations, in which they drop from further consideration certain members of their initial ensemble and communicate classically between them to ensure agreement about which particle pairs are dropped.
   - *Adding an uncorrelated ancilla.* Each party can add another quantum system – the so-called ancilla – to his ensemble of systems. The ancilla must be uncorrelated in the sense that it is not entangled in any way to the ensemble of the other party.
2. Classical communication.
   This allows for the opportunity to classically correlate the actions of the two parties by both one-way and two-way communication. These are any completely positive linear and trace-preserving maps of the density operator that can be implemented locally by classical coordination among the parties. For example party A could perform local measurements on his particles and communicate to B his results so that B can coordinate his local operations with the outcomes A gets from his operations. However, party A is not allowed to exchange any quantum systems nor to perform any nonlocal operation. (In contrast, non-classical communication uses specific quantum correlations or entanglement assisted communication such as teleportation.)

This specification of LOCC is still rather ambiguous and thus not very precise. Especially the idea of classical communication is hard to formalize, and the above presentation is even circular. For more clarity we better ask what transformations defined at an operational level are represented by LOCC. But before specifying this special case I will first treat general quantum dynamics.

[3]Sometimes abbreviated as LQCC.

General quantum dynamics can be represented mathematically by completely positive linear maps that do not increase the trace [80]. Such a map $\mathcal{L}$ is written as $\mathcal{L}(\rho) = \sum_i L_i \rho L_i^\dagger$, where $\sum_i L_i L_i^\dagger \leq \mathbb{1}$. The equality holds for trace preserving super operators. These correspond physically to non-selective dynamics. In general the super operators may be trace decreasing and correspond to selective operations, e.g. a measurement followed by a selection of systems depending of the outcome. The special quantum dynamics generated through LOCC can now be properly defined as follows:

Definition 3.1.2. *Local operations and classical communication (LOCC) is represented by a* multi-local super operator*, i.e. by a completely positive linear map $\mathcal{L}$ that does not increase the trace: $\mathcal{L}(\rho) = \sum_i L_i \rho L_i^\dagger$, where $\sum_i L_i L_i^\dagger \leq \mathbb{1}$, and the L_i's are products of local operators for the parties A, B, etc. : $L_i = L_i^A \otimes L_i^B \dots$ [80].*[4]

From this definition it follows that any LOCC operation on a bi-partite state can be written as:

$$\rho \longrightarrow \rho' = p \sum_i (L_i^A \otimes L_i^B) \rho (L_i^A \otimes L_i^B)^\dagger, \tag{3.6}$$

where $p \leq 1$ is a normalization constant interpreted as the probability of realizing the operation. For $p < 1$ one refers to *s*tochastic local operations and classical communication (SLOCC)

Now, using this definition, we are able to interpret the separability of quantum states by means of the (intuitive) idea that local operations and classical communication (LOCC) cannot have non-local effects. This proceeds as follows. Suppose that the two parties A and B are in the possession of arbitrary unentangled states ρ^A and ρ^B from a certain set of states. These parties perform any possible LOCC operation $\mathcal{L}$ on their states. This means that the original combined system $\rho = \rho^A \otimes \rho^B$ is transformed into $\mathcal{L}(\rho)$ as follows:

$$\begin{aligned} \mathcal{L}(\rho) &= p \sum_i L_i (\rho^A \otimes \rho^B) L_i^\dagger = p \sum_i (L_i^A \otimes L_i^B)(\rho^A \otimes \rho^B)(L_i^A \otimes L_i^B)^\dagger \\ &= p \sum_i L_i^A \rho_i^A L_i^{A\dagger} \otimes L_i^B \rho_i^B L_i^{B\dagger} = p \sum_i \tilde{p}_i \tilde{\rho}_i^A \otimes \tilde{\rho}_i^B \end{aligned} \tag{3.7}$$

The remarkable thing about the final composed state $\tilde{\rho}$ parties A and B can produce is that it is again a separable state !

This result gives us the conclusion that the only states the two parties A and B can produce using LOCC are the separable states (i.e. classical mixtures) of Eq. (3.4) and they can thus not create any entanglement by using only LOCC. This provides evidence for the intuitive idea that local operations and classical communication (LOCC) cannot have non-local effects.

[4] So far no practical criterion exists that determines whether a generic transformation $\mathcal{L}$ can be implemented by means of LOCC [69].

3.2 Definition and Classification of Entangled Quantum States

In this section the non-separable states or entangled states will be defined and classified through their entanglement properties, not only for bi-partite systems but for a finite but otherwise arbitrary number of systems. However, this will not be a complete investigation because the description of the entanglement (and distillability) properties of systems with more than two parties is still very much under investigation [67].

First I will discuss bi-partite systems and the notion of maximal entanglement for these systems. Then I will generalized this notion. First to three systems where two different types of tri-partite entanglement can be distinguished and subsequently to N-partite systems.

3.2.1 Bi-partite Systems. What is Maximal Entanglement?

Let us recall the formal definition of bi-partite entanglement.

Definition 3.2.1. *Two quantum systems labeled A and B are called entangled when the composed state ρ^{AB} cannot be factorised into a convex sum of product states:*

$$\rho^{AB} \neq \sum_i p_i \; \rho_i^A \otimes \rho_i^B \tag{3.8}$$

with $\sum_i p_i = 1$.

For pure states this reduces to the following. The composite state $|\,\Psi\rangle^{AB}$ is entangled iff it cannot be factorised into two separate states $|\,\psi\rangle^{A}$ and $|\,\phi\rangle^{B}$:

$$|\,\Psi\rangle^{AB} \neq |\,\psi\rangle^{A} \otimes |\,\phi\rangle^{B} . \tag{3.9}$$

All possible states $|\,\Psi\rangle^{AB}$ of the composite system form a set $\mathcal{S}$. In general these states are entangled; only in *rare* cases is the state separable. The set of separable states forms a subset of $\mathcal{S}$ with measure zero, and the set of maximally entangled states also forms a subset of $\mathcal{S}$ with measure zero [51]. The definition of maximal entanglement for two finite-dimensional systems is as follows:

Definition 3.2.2. *Two systems A and B are called maximally entangled when their composed state $|\,\Psi\rangle$ in the Schmidt decomposition can be written as*

$$|\,\Psi\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{i=N} |\,\phi_i\rangle \otimes |\,\psi_i\rangle \tag{3.10}$$

with $\{|\,\phi_i\rangle^A\}$ and $\{|\,\psi_i\rangle^B\}$ two orthonormal bases on $\mathcal{H}^A$ and $\mathcal{H}^B$ with dimension d_A and d_B. Here N is equal to the smallest dimension.

As an example, suppose we have two two-level systems 1 and 2 whose states can be written in the orthonormal basis $\{|\uparrow\rangle , |\downarrow\rangle\}$. Physically, these systems could be for example electrons in a magnetic field or polarized photons. Every composed state of the two systems together can be written on the basis of four orthogonal states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$. Together these basis states generate a four-dimensional Hilbert space. But this basis is not unique. Another possible orthonormal basis for this space is the so-called *Bell basis* and is given by the following *Bell states*:

$$\begin{aligned} |\Psi^{\pm}\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle), \\ |\Phi^{\pm}\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle). \end{aligned} \tag{3.11}$$

These Bell-states are examples of maximally entangled states. These are not the only maximally entangled states but they are a convenient and common choice to represent maximally entangled states.

3.2.2 Tri-Partite Systems.

The bi-partite entangled states of the previous section can be extended to three parties. Accordingly, we could define a tri-partite state to be entangled iff it cannot be written as a convex sum of tri-partite product states. However, we also have to consider the possibility bi-partite entanglement in tri-partite systems. Therefore, the following definition of full tri-partite entanglement has to be adopted:

Definition 3.2.3. *A state ρ is called* fully tri-partite entangled *iff no convex decomposition of the form*

$$\rho = \sum_i p_i \rho_i, \qquad \textit{with } p_i \geq 0,\ \textstyle\sum_i p_i = 1, \tag{3.12}$$

exists in which all the states ρ_i are factorisable into products of states of less than three parties.

This definition excludes the fully separable states ($\rho = \rho_A \otimes \rho_B \otimes \rho_C$) and the bi-separable states (e.g. $\rho = \rho_{AB} \otimes \rho_C$). See figure 3.1.

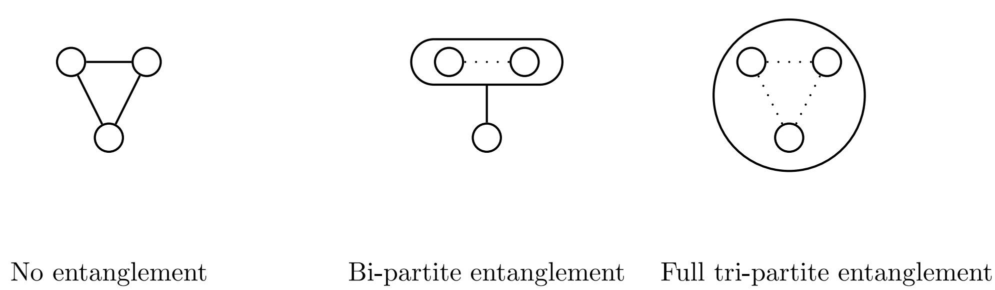


Figure 3.1: Types of entanglement in tri-partite systems.

For instance, the so-called Greenberger-Horne-Zeilinger- or GHZ-state defined as

$$|\psi\rangle_{GHZ} = (|\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\rangle)/\sqrt{2}, \tag{3.13}$$

is a fully entangled tri-partite state. On the other hand, the three-particle state

$$\rho = \frac{1}{2}(\widehat{P}_{\uparrow}^{(1)} \otimes \widehat{P}_{S}^{(23)} + \widehat{P}_{\downarrow}^{(1)} \otimes \widehat{P}_{T}^{(23)}) \tag{3.14}$$

is only two-particle entangled. Here, $\widehat{P}_{T}^{23)}$ and $\widehat{P}_{S}^{(23)}$ denote projectors on the triplet state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ and singlet state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ respectively for particles 2 and 3, and $\widehat{P}(1)_{\downarrow} = |\downarrow\rangle\langle\downarrow|$ and $\widehat{P}_{\uparrow}^{(1)} = |\uparrow\rangle\langle\uparrow|$ are the 'down' and 'up' states for particle 1.

The GHZ-state of Eq.(3.13) can be thought of as a Schmidt decomposition for three systems (i.e. it can be written as a single sum over orthonormal basis states: $|\psi\rangle = \sum_i \frac{1}{\sqrt{i}} |i, i, i\rangle\,, \; i \in \mathbb{N}^+$). Contrary to the bi-partite case it is not true that such a Schmidt-decomposition exists for any pure tri-partite state.

This has the consequence that for multi-partite systems entanglement can no longer be defined in terms of the Schmidt decomposition and there is no analogous definition of maximal entanglement. Thus in this respect tri-partite entanglement differs genuinely from bi-partite entanglement.

For example the so called W-states

$$|\psi\rangle_W = (|\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle)/\sqrt{3}, \tag{3.15}$$

cannot be written in terms of the Schmidt decomposition as in Eq.(3.13), although it represents three fully entangled systems. The reason is that the number of linear independent terms exceeds the number of orthonormal basis states of the separate systems. [51].

In fact, Dür *et al.* have proven that a single copy of a tri-partite entangled state (two-level systems) can be transformed either to the state $|\psi\rangle_{GHZ}$ or to the state $|\psi\rangle_W$ by stochastic local operations and classical communication (SLOCC) [69]. Here stochastic LOCC means that it is through LOCC but without posing that it has to be achieved with certainty.

Thus under SLOCC, the states $|\psi\rangle_{GHZ}$ and $|\psi\rangle_W$ generate two equivalence classes, i.e. two distinct subsets of the total Hilbert space ($\mathcal{H}_2^{\otimes 3}$) spanned by the three two-level systems [51]. In other words, the state space of single tri-partite systems has two different types of locally inequivalent maximally entangled states[5]. These equivalence classes are represented in figure 3.2.

The state $|\psi\rangle_W$ and $|\psi\rangle_{GHZ}$ can be said to differ from each other not only because they cannot be obtained from each other by means of SLOCC, but also because they differ in an interesting way when we consider entanglement properties of the respective subsystems. If one of the three parties in the GHZ-state is traced out, the remaining bi-partite state is completely unentangled. Thus any reduced density operator is a separable state. The entanglement properties are thus very 'fragile' under disposal of particles. However, oppositely, the W-state is maximally 'robust' under disposal of any one of the three particles, in the sense

[5]The possibility to convert under SLOCC an entangled state into another has lead to defining equivalence relations in the set of entangled states, and also to establishing hierarchies between the resulting classes. Two different types of classifications should not be confused. One could consider the transformation properties of a set of *many* copies of a particular state (asymptotic results), or alternatively one could consider the transformation properties of only *single* copies of the same state. See Ref. [69] for a detailed investigation.

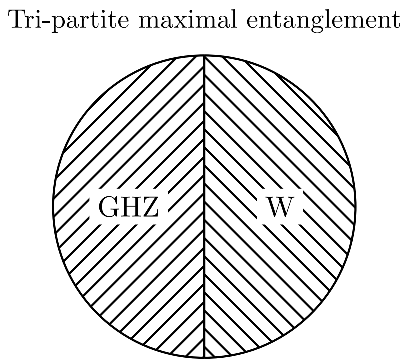


Figure 3.2: Equivalence classes of tri-partite maximally entangled states under SLOCC.

that the remaining reduced density operators ρ^{AB}, ρ^{AC} and ρ^{BC} are maximally entangled bi-partite states. Thus $|\,\psi\rangle_W$ can be said to be robust and $|\,\psi\rangle_{GHZ}$ to be fragile under particle disposal.

The above mentioned classification of tri-partite entangled states in the GHZ- and W- types is only for *pure* states. An analogous classification of *mixed* tri-partite states is currently being investigated [70], but will here not be further commented on. Furthermore, the tri-partite case has been extended to the four-partite case. Using four-partite quantum systems composed out of four qubits, similar results have been achieved as in the tri-partite pure case, i.e. the behavior of a single copy of a pure four-partite state under the action of SLOCC has been classified. In this case we have not two but nine different equivalence classes generated by the group of reversible SLOCC operations, corresponding to nine different ways of entangling four qubits [79].

3.2.3 N-partite Entanglement

The discussion of entanglement now be further extended to include a finite but otherwise unrestricted amount of systems labeled by N. This extension has been done in collaboration with Uffink [93].

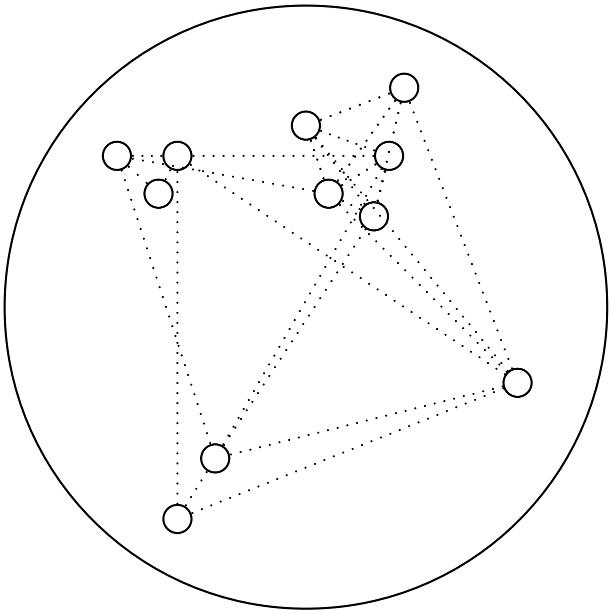
I start with the definition of the basic concept.

Definition 3.2.4. *Consider an arbitrary N-partite system described by a Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N$. A general mixed state ρ of this system is called* fully *N-partite entangled iff no convex decomposition of the form*

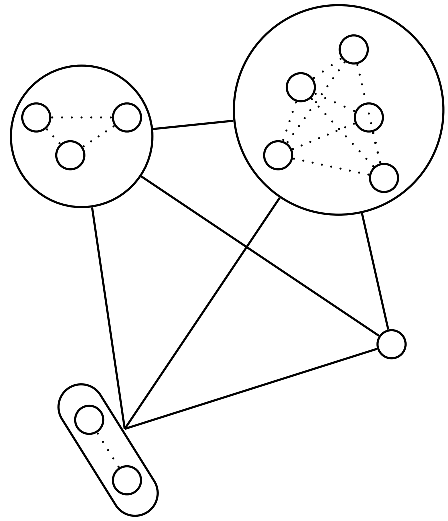
$$\rho = \sum_i p_i \rho_i, \qquad \textit{with } p_i \geq 0,\ \textstyle\sum_i p_i = 1, \tag{3.16}$$

exists in which all the states ρ_i are factorisable into products of states of less than N parties.

Of course, since each separable mixed state is a mixture of separable pure states, one may equivalently assume that separable states ρ_i are pure, so that the de-



Full entangled 11-particles state.



5-particle entangled 11-particles state.

Figure 3.3: Types of N-partite entanglement.

composition of Eq.(3.16) takes the form

$$\rho = \sum_i p_i \,|\, \psi_i \rangle \, \langle \psi_i | \, . \tag{3.17}$$

In order to extend the above terminology, let K be any subset $K \subset \{1, \ldots , N\}$ and let ρ^K denote a state of the subsystem composed of the parties labeled by K.

Definition 3.2.5. *An N-partite state is called M-*partite entangled *($M < N$) iff the following form of* partial separability *holds, i.e. iff a decomposition exists of the form*

$$\rho = \sum_i p_i \, \rho_i^{K_1^{(i)}} \otimes \cdots \otimes \rho_i^{K_{r_i}^{(i)}} , \tag{3.18}$$

where for each i, $K_1^{(i)}, \ldots , K_{r_i}^{(i)}$ is some partition of $\{1, \cdots N\}$ into r_i disjoint subsets, each subset $K_j^{(i)}$ containing at most M elements; but no such decomposition is possible when all these subsets are required to contain less than M elements.

All N-particle M-partite entangled states with $M < N$ are called *non-fully entangled states* or *partially separable states.* See figure 3.3.

An example of a N-partite state which is fully N-partite entangled is the generalized Greenberger-Horne-Zeilinger-state

$$|\, \psi^N_{\mathrm{GHZ}} \rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\uparrow \cdots \uparrow\rangle + |\downarrow\downarrow \cdots \downarrow\rangle \right) . \tag{3.19}$$

And as an example of a N-partite state that is $(N-1)$-partite entangled consider the tri-partite entangled four-particle state:

$$|\,\Psi\rangle = |\uparrow\rangle \otimes |\,\psi^3_{\mathrm{GHZ}}\rangle\,. \tag{3.20}$$

Note that, as the tri-partite state (3.14) exemplifies, an N-partite state can be M-partite entangled even if it has no M-partite subsystem whose (reduced) state is M-partite entangled.

3.2.4 Quest for N-partite Classification

N-partite entanglement is far from being completely classified. The classification of arbitrary states is often simplified to the classification of certain special family of states which have certain symmetries or special properties. For example, Ziman *et al.* [66] divide the total Hilbert space in the following way : $\mathcal{H}_{1\ldots N} = \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_N = \mathcal{H}_X \otimes \mathcal{H}_Y$, where X and Y are two sets of subsystems. And Dür and Cirac [67] give a classification of N-partite two-level systems in terms of their partitions. In particular, they consider k-partite splits, i.e. partitions dividing a N-partite systems into $k \leq N$ parties. This gives rise to a whole hierarchy of different classes. They furthermore use a specific class of states, containing also the GHZ- and W-states in the tri-partite case, for which more definite results can be obtained. However these investigations have not yet been completed and will therefore not be considered here.

3.2.5 Fidelity

In the context of information theory it is important to have measures of information. One such measure is the *fidelity* which is used to specify the amount of information that can be gained from a measurement on a quantum bit when the state of the system is not known beforehand [51, 74]. The fidelity of a state ρ with respect to the pure state $|\,\phi\rangle$ is defined as

$$F(\rho) = \langle\,\phi|\,\rho\,|\,\phi\rangle\,. \tag{3.21}$$

Although the fidelity was originally introduced in estimation theory, it can also be used for other purposes. For example, certain bounds on the fidelity measure F can be used as a sufficient criterium for certain types of entanglement. One such criterium will be here explicitly formulated because it will be needed in the remainder of this thesis.

The issue concerned is the discrimination of full N-partite entanglement (see section 3.2.3) from lesser forms of entanglement in N-partite systems. A sufficient condition for this discrimination of full N-particle entanglement that uses the fidelity measure is now presented[93]. It follows from the fact that the internal correlations (i.e. the entanglement) of a quantum state are encoded in the off-diagonal elements of the density matrix that represents the state in a product basis. I summaries here the derivation presented by Sackett *et al.* [74]. They consider the state preparation fidelity F of a N-particle state ρ defined as

$$F(\rho) := \langle\psi_{\mathrm{GHZ}}|\rho|\psi_{\mathrm{GHZ}}\rangle = \frac{1}{2}(P_\uparrow + P_\downarrow) + \mathrm{Re}\;\rho_{\uparrow\downarrow}, \tag{3.22}$$

where $|\,\psi_{\rm GHZ}\rangle$ is given by (3.19), $P_\uparrow := \langle \uparrow \cdots \uparrow|\,\rho\,|\uparrow \cdots \uparrow\rangle$, $P_\downarrow := \langle \downarrow\downarrow \cdots \downarrow|\,\rho\,|\downarrow\downarrow \cdots \downarrow\rangle$ and $\rho_{\uparrow\downarrow} := \langle \uparrow\uparrow \cdots \uparrow|\,\rho\,|\downarrow\downarrow \cdots \downarrow\rangle$ is the far off-diagonal matrix element in the z-basis. Now partition the set of N particles into two disjoint subsets K and K' and consider a pure state of the form

$$|\,\phi\rangle = \left(a\,|\uparrow\uparrow \cdots \uparrow\rangle^K + \cdots + b\,|\downarrow\downarrow \cdots \downarrow\rangle^K\right) \otimes \left(c\,|\uparrow\uparrow \cdots \uparrow\rangle^{K'} + \cdots + d\,|\downarrow\downarrow \cdots \downarrow\rangle^{K'}\right) \tag{3.23}$$

where $|\uparrow\uparrow \cdots \uparrow\rangle^K$ is the state with all particles in subset K in the 'up'-state and similarly for the other terms. Normalization of $|\,\phi\rangle$ leads to $|a|^2 + |b|^2 \leq 1$ and $|c|^2 + |d|^2 \leq 1$. It then follows that

$$\begin{aligned} 2F(|\,\phi\rangle\,\langle\,\phi|) &= |ac|^2 + |bd|^2 + 2\mathrm{Re}\,(ab^*cd^*) \\ &\leq \left((|a|^2 + |b|^2\right)\left(|c|^2 + |d|^2\right) \leq 1. \end{aligned} \tag{3.24}$$

Thus, the state preparation fidelity is at most 1/2 for any state of the form (3.23). From the convexity of $F(\rho)$ it follows that this inequality also holds for any mixture of such product states, i.e. for any state ρ as defined in Eq. (3.17).

A sufficient condition for N-particle entanglement is thus obtained, namely

$$F(\rho) > 1/2. \tag{3.25}$$

Of course, analogous conditions can be obtained by replacing the special state $|\,\psi_{\rm GHZ}\rangle$ in definition (3.22) by another maximally entangled state, such as $\frac{1}{\sqrt{2}}(|\uparrow \ldots \uparrow\downarrow\rangle \pm |\downarrow \ldots \downarrow\uparrow\rangle)$ etc.

An experimental test of this condition requires the determination of the real part of the far off-diagonal matrix element $\rho_{\uparrow\downarrow}$. Of course, Re $\rho_{\uparrow\downarrow}$ is not the expectation value of a product observable, and information about this quantity can only be obtained indirectly. Experimental procedures by which this information can be obtained have to make sure that no unwanted matrix elements contribute to the determination of this quantity.

3.3 The Distillability Problem

In this section I will discuss the idea of *distillation* or *purification* of quantum states and will show the relationship between distillability properties and the separability properties of the previous section.

In section 3.1 I have introduced the Werner states which possess a local hidden variable model for any projective measurements but which are not separable. These states do not violate any Bell inequality for usual projective measurements, but do show violation if subjected to a sequence of local measurements or to so-called local collective operations. This feature is the so called 'hidden entanglement' [52] and as mentioned before will be a central topic in some later sections. But this *same* feature has motivated the question of *distillability*: Can we get a maximally entangled state (that violates a Bell-inequality maximally) from another entangled mixed state (that perhaps does not violate any Bell inequality such as the Werner state) trough local operations and classical communication? In other words, is it possible to 'distill' or 'purify' a collection of quantum states trough certain local operations or classical communication (LOCC) to obtain a maximally entangled state? This idea of distillation has its origins in quantum information theory. For many applications in quantum information processing and communication one needs a maximally entangled state, although very often this state is not available but has to be 'distilled' from an ensemble of non-maximally entangled states.

These maximally entangled states in an $M \times N$, $(M < N)$ dimensional space are the states that can be brought by a local change of basis to the form [59]:

$$|\,\Psi_{max}\rangle = \frac{1}{\sqrt{M}} \sum_{i=0}^{i=M} |\,\phi_i\rangle \otimes |\,\psi_i\rangle \tag{3.26}$$

with $\{|\,\phi_i\rangle\}$ and $\{|\,\psi_i\rangle\}$ two orthonormal bases. How can two parties come into the possession of a maximally entangled state? Although in principle one can create pure and maximal entangled states, in real life any pure state will evolve to a mixed state due to interactions with the environment. As an example consider two initially maximally entangled particles (e.g. photons) which are send to the two parties through a noisy channel. In order to obtain maximally entangled states again, the idea of distillation or purification becomes relevant, i.e. using only local operations and classical communication (LOCC) the parties A and B try to obtain maximal entanglement from the non-maximally entangled mixed state. That is, is it possible using LOCC to transform $\rho \otimes^N \rho$ to a supply of maximally entangled states? Here the $\otimes^N$ notation indicates that N copies of the mixed state ρ are available. For Hilbert spaces of bi-partite systems of total dimension lower or equal to 6, any mixed entangled state can always be distilled to its pure form [63]. As we have already seen, entanglement for these systems is equivalent to the NPPT-property. Therefore, for 2×2 and 2×3 systems all NPPT-states are distillable. However, the Horodecki's [64] showed that for higher dimensional systems there exist entangled states, termed as *bound entangled states* which cannot be distilled, in contraposition to *free entangled states* which can be distilled.

As we will see, this distillation of entanglement is neither rare nor ubiquitous; some bi-partite mixed states ρ can be successfully distilled and some cannot [71]. Much work has been focussed on whether ρ falls into the distillable or undistillable class, although the problem has not yet been completely resolved. The distillability problem can now thus be formulated as follows: *Given a density matrix ρ is it or is it not distillable?*

In order to investigate this problem, let me first define the distillability property. I will follow the approach of Lewenstein *et al.* [59] by first giving an intuitive account of distillability and then present the definition.

The intuitive idea is that ρ is distillable if by performing LOCC on an arbitrary number N of copies ρ, parties A and B can get a two-particle maximally entangled state $|\,\Psi_{max}\rangle$[6]:

$$\rho \otimes \ldots \otimes \rho \longrightarrow |\,\Psi_{max}\rangle\,\langle\,\Psi_{max}|\,. \tag{3.27}$$

[6] An alternative definition which is sometimes used, makes reference of distillation to *any* entangled pure state instead of to maximally entangled states [72].

This formulation requires the specification of what LOCC can do with N copies of ρ. This is not an easy job, and therefore this definition does not lead to a practical criterium for distillability. Fortunately, according to a theorem of Ref.[64] a much more practical definition exists. Instead of studying the whole set of possible LOCC procedures, in order to study the distillability of a given density operator, it is sufficient to only study projections onto a 2×2-dimensional subspace of the total Hilbert space of ρ. This theorem reduces the problem of distillability to a very precise mathematical question.

Before presenting the general definition I first have to treat the distillability of 2×2 systems. Any entangled 2×2 system has the entanglement that can be distilled to singlet form. Thus using LOCC on a supply of entangled states singlet states can be obtained. This was proven by Ref.[63] using a specific protocol to obtain a non-zero number of singlet states out of a collection of entangled 2×2 states. I will not discuss the specific details of the protocol that was used. Recall that any 2×2 entangled state is NPPT. I then follows that for 2×2 states NPPT implies distillability.

The general definition of distillability uses this 2×2 result:

Definition 3.3.1. *ρ is distillable iff there exists a number of copies N, and a projector $P_{2\times2}$ onto a 2×2-dimensional subspace spanned by*

$$\begin{aligned} |\,\alpha_i\rangle \;\; &\in \underbrace{\mathcal{H}_A \otimes \ldots \otimes \mathcal{H}_A}_{N-times}, \quad i = 1,2 \\ |\,\beta_i\rangle \;\; &\in \underbrace{\mathcal{H}_B \otimes \ldots \otimes \mathcal{H}_B}_{N-times}, \quad i = 1,2 \end{aligned} \tag{3.28}$$

such that the 2×2 state $\sigma = P_{2\times2}\rho^{\otimes N}P_{2\times2}$, is NPPT and therefore distillable.

This definition can be understood by the following alternative formulation: ρ is distillable iff there exists a state $|\,\psi\rangle$ of a 2×2-dimensional subspace

$$|\,\psi\rangle = a\,|\,\alpha_1^*\rangle\,|\,\beta_1\rangle + b\,|\,\alpha_2^*\rangle\,|\,\beta_2\rangle \tag{3.29}$$

such that $\langle\,\psi|\,(\rho^{T_A})^{\otimes N}\,|\,\psi\rangle < 0$ (i.e. this state is NPPT) for some number of copies N.

What is the idea behind this definition? If ρ is distillable it means that a maximally entangled state can be produced. This state can be easily projected using local operations onto a pure state in a 2×2-dimensional subspace. On the other hand, suppose we have a state $|\,\psi\rangle$ as in Eq.(3.29), such that $\langle\,\psi|\,\rho^{T_A}\,|\,\psi\rangle < 0$, then one can first project ρ onto the 2×2 subspace to which $|\,\psi\rangle$ belongs. This is a 2×2 subspace in which the projected density operator ρ is NPPT, and therefore from theorem 3.1.2 it is entangled and furthermore it is distillable (Recall that for 2×2 and 2×3 systems all NPPT-states are distillable.) [59].

A procedure that succeeds in distillation of a certain state is called a distillation or purification *protocol*. As an example I will consider the very first distillation protocol [1], called the BBPSSW protocol after its inventors. Consider two parties A and B sharing the following Werner state ρ_W,

$$\rho_W = \epsilon\,\big|\,\Psi^-\big\rangle_{12}\big\langle\,\Psi^-\big| + \frac{1-\epsilon}{4}\mathbb{1}, \tag{3.30}$$

with $|\Psi^-\rangle_{12}$ the bi-partite singlet state, one of the Bell states of Eq. (3.11). For $\epsilon < 1$ this is not a maximally entangled state, it has a fraction F of singlet states equal to

$$F = \frac{1+3\epsilon}{4}.$$

In order to distill this state consider two systems each in a Werner state. The total state of the systems is $\rho_W \otimes \rho_W$. As a first step party B operates the Pauli operator σ_{2y} on his part of the system. This amounts to the swapping $\Psi^\pm \leftrightarrow \Phi^\pm$ in the Bell basis [51]. Next party B applies the *controlled NOT* to his two subsystems after which both parties measure the resulting target state in the product basis.[7] They compare their outcomes using classical communication and if the outcomes match, party B again performs the operator σ_{2y} on his remaining subsystem. After a successful run both parties share a single state ρ'_W with a fraction F' of singlet states equal to

$$F' = \left\langle \Psi^- \middle| \rho_W \middle| \Psi^- \right\rangle = \frac{1+2\epsilon+5\epsilon^2}{4+4\epsilon}. \tag{3.31}$$

For $\epsilon > 1/3$ we get $F' > F$ and the fraction of singlets increases. By iterating the procedure one can get an arbitrary high fraction. But the larger F is required the more particles are sacrificed and the less the probability of success is.

3.3.1 Distillability Related to Separability.

What is the relationship between the criterium of partial transposition (which plays such an important role in the separability problem) and the distillability problem? In other words, how do separability properties of a state ρ relate to its distillability properties? The following two theorems summarize the as yet known results:

Theorem 3.3.1. *If $\rho^{T_A} \geq 0$ (ρ is PPT) then ρ is not distillable [64].*

Theorem 3.3.2. *If $\rho^{T_A} < 0$ (ρ is NPPT) in dimensions $2\times 2,\ 2\times 3$ and $2\times N$ then ρ is distillable [69].*

From these two theorems we see that the set of PPT density operators, even those which are entangled, are not distillable. These states, in which entanglement is present but cannot be extracted, are said to have *bound entanglement*. Thus bound entangled states are entangled states that cannot be distilled to a maximally entangled state; the entanglement is 'bound' and not 'free'. The PPT/NPPT classification of density operators used in the separability problem has led to a recent conjecture about distillability, namely that all states with NPPT are distillable (or equivalently, that all non-distillable states are PPT states). This conjecture has as yet not been proven. In fact, in Ref. [71] this

[7] The *controlled NOT* is the following unitary operation

$$U_{controlled\ NOT}\,|i\rangle\,|j\rangle = |i\rangle\,|(i+j)mod2\rangle.$$

The first state is called the source, the second the target.

conjecture is itself conjectured to be false: strong evidence is presented that a certain family of states has only bound entanglement (entangled but not distillable) despite being NPPT.

In order to summarize the above mentioned results, relating the separability properties of a state ρ to its distillability properties, I represent them in figures 3.4, 3.5 and 3.6.

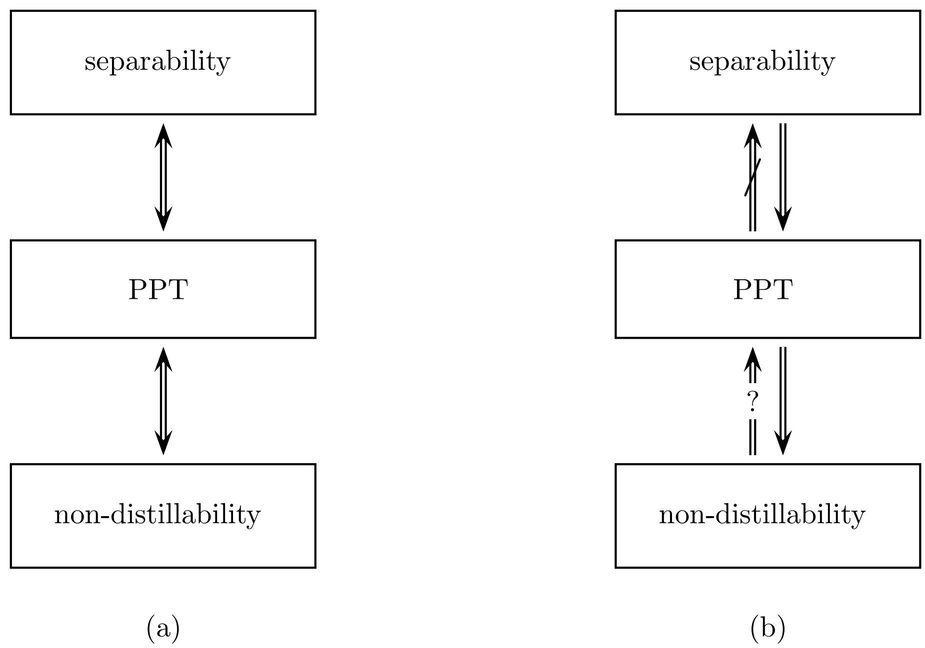


Figure 3.4: Separability related to distillability: (a) dimension 2×2 and 2×3, (b) general dimension $M \times N$. The '?' indicates the as yet unproven conjecture that all NPPT states are distillable (or equivalently, that all non-distillable states are PPT states).

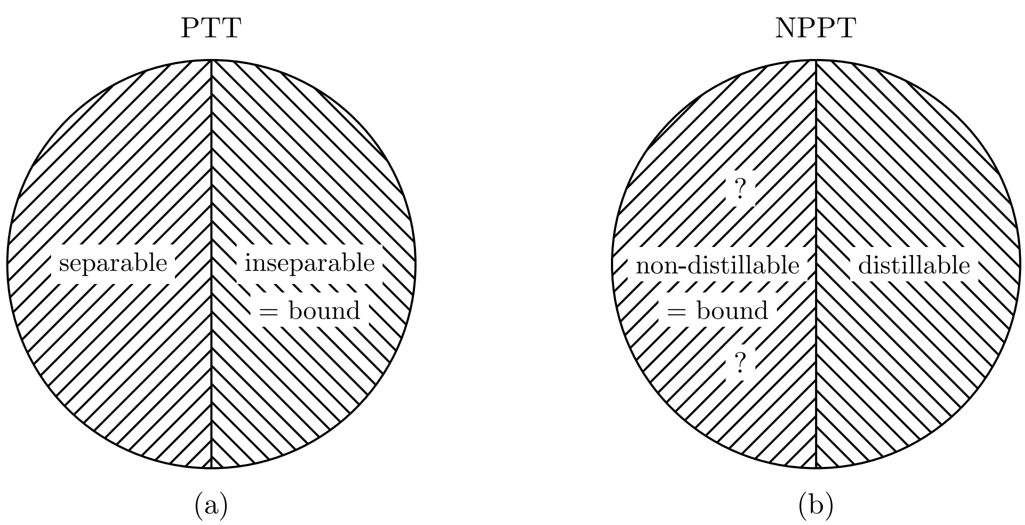


Figure 3.5: Separability related to distillability. Venn-diagram of the set of all bi-partite mixed states ρ: (a) PPT states, (b) NPPT states. The '?' indicates the conjectured region of bound entanglement. This region does not contain any states for $2 \times N$ [71].

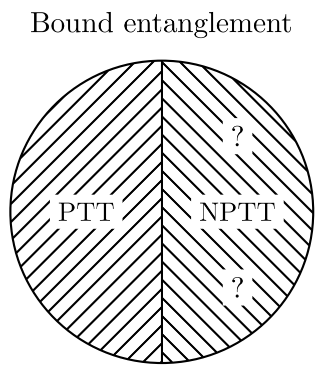


Figure 3.6: Bound entanglement. The NPTT region has been conjectured.

3.4 Classification of Quantum States. Part II. Classification through entanglement.

In this chapter the entanglement properties of quantum states have been examined. This has lead to the distinction of certain sets of quantum states with specific characteristics. This allows for an extension of the classification of the total quantum mechanical state space presented in section 2.6, i.e. a classification through entanglement properties and through information theoretic considerations. For brevity the newly distinguished states will not be fully described, only the sections in which they appear are referred to.

- PPT-states and NPPT-states. Section 3.1.2.
- Free entangled states. Also called distillable entangled states. Section 3.3.1.
- Bound entangled states. Also called non-distillable entangled states. Section 3.3.1.
- Maximally entangled bi-partite states. Section 3.2.1.
- Tri-partite entanglement: GHZ-, W-states. Section 3.2.2.
- Full N-particle entangled states. Section 3.2.3.
- M particle entangled N-particle states ($M < N$. Also called partially separable states. Section 3.2.3.

3.5 Conclusion and Summary

In this chapter I have considered quantum entanglement. Because an entangled state is defined as a non-separable state the separability properties of density operators have been discussed. The partial transpose criterium is shown to give a necessary criterium for separability, and for small Hilbert spaces a sufficient criterium as well. The structure of the bi-partite, tri-partite and N-partite entangled state space has been reviewed and specific distinctions such as maximal and full entanglement have been made. The family of entangled states (pure and mixed) is investigated to see whether or not they can be distilled or purified to specific pure states (i.e. the maximally entangled states). In doing so I had to define what is meant by local operations and classical communication (LOCC). The distillability and separability properties of quantum states have been related to each other. The implicative connections between separable, positive partial transpose, and non-distillable states have been formulated and are shown in specific figures. It was found that separability implies positive partial transposition, although the converse is not true for all states. Positive partial transposition in turn implies non-distillability. Whether the converse holds –i.e. whether non-distillability implies positive partial transpose– is not yet known. However, for bi-partite two-dimensional systems all three concepts imply each other.

Lastly, the classification of the quantum state space as given in chapter 2 has been extended by a second classification, i.e. through entanglement properties and aspects of quantum information. Here all the quantum states that have been distinguished in this chapter are listed.

Chapter 4

Local Hidden Variable Theories, Bell Theorems and derivation of the Bell-inequalities

Whereas in the last chapter the separability aspect of quantum states was studied, in this chapter the locality aspect will be investigated. In the next chapter these two aspects will be explicitly compared to each other.

This chapter will start in section 4.1 with a consideration of the question of the completeness of quantum mechanics as formulated in the so-called 'hidden variables program'. Further, it addresses the various Bell-type theorems that state that such a program is impossible.

The hidden variables formalism and the derivation of Bell's inequality and the Bell-theorem are treated extensively in the following section 4.2 to set the terminology for future sections. This section acts also as preliminary information and is in part historical to get a better understanding of the issue concerned. Only simple two particle systems are considered.

In section 4.3 more complex bi- and tri-particle systems are considered in the construction of Bell-theorems. This leads to new *Gedankenexperiments*, the so-called Bell-theorems without inequalities and algebraic proofs. These are compared to the original Bell-theorem for logical strength and experimental testability.

In section 4.4 the extension is made from the bi-partite case to the N-partite case both for full factorisability and for the specific locality hypothesis of partial factorisability. Here the Bell-type inequalities for full factorisability are extended to complete sets (i.e. to necessary and sufficient sets) of Bell-type inequalities for local realism to hold. Furthermore, the extension to the specific locality hypothesis of partial factorisability results in new Bell-type inequalities, the so-called Svetlichny inequalities, and in a new type of hidden variable theories, the so-called Partial Local Hidden Variables Theories (PLHV).

Finally, all these considerations are confronted with the structure of the quantum mechanical state space and consequently an extension is given of the two classifications of quantum states of the previous two chapters. This is a classification through factorisability and hidden variables simulability and is presented in section 4.6, the last section of this chapter.

4.1 Introduction to incompleteness, non-locality and realism[1].

> "Theoretical physicists live in a classical world, looking out into a quantum mechanical world.... Now nobody knows just where the boundary between the classical and quantum domain is situated. Most feel that the experimental switch setting and pointer readings are on this side. But some would think the boundary nearer, others would think it farther, and many would prefer *not* to think about it." [20]

> "To know the quantum mechanical state of a system implies, in general, only statistical restrictions on the results of measurement, It seems interesting to ask if this statistical element be thought of as arising, as in classical statistical mechanics, because the states in question are averages over better defined states for which individually the results would be quite determined. These hypothetical 'dispersion free' states would be specified not only by the quantum mechanical state vector but also by additional 'hidden variables'- 'hidden' because if states with prescribed values of these variables could actually be prepared, quantum mechanics would be observable inadequate." [16]

These quotes are from the introduction of two papers of John Bell's famous collection of papers. This collection deals with the long debated question whether or not quantum mechanics is a complete physical theory, i.e. it addresses the so-called incompleteness problem:

Definition 4.1.1 (Incompleteness problem, preliminary formulation). *"Is quantum mechanics a complete physical theory?"*

By a complete physical theory is meant the following. Does quantum mechanics give an exhaustive description of the physical phenomena? Being still ambiguous, this formulation of the incompleteness problem is only preliminary. It will be ever more made explicit and restrictive in the following sections. Before presenting this, let me try to make this incompleteness problem a little more concrete.

One way to make this incompleteness problem more concrete is to ask if hypothetical quantities referred to as 'dispersion free states' or more well known as 'hidden variables' can be used to complete the theory[2]. Following John Bell [20], the overall motivation to study hidden variables – as an attempt to answer the incompleteness problem – can be distinguished into three distinct motivations.

1. The prospect of a *unitary account* of the world and the wish to dispense with the dichotomy of the physical world into classical and quantum mechanical phenomena. John Bell put it as follows: "It is this possibility, of a homogeneous account of the world, which is for me the chief motivation of the study of the so-called 'hidden-variable' possibility [20]".

[1] This is the title of the very valuable book of Redhead [46]

[2] Not everybody agrees that this is a fruitful way to answer the incompleteness problem. Some want a completely new theory not just a refinement. See also footnote 3 about Einstein's position in this debate.

2. To get rid of the statistical element of quantum mechanics and get some form of *realism* and/or *determinism* back into the realm of micro physics. Physical objects then can be assigned some sort of objective set of properties whose behavior could be principally determined by physical laws.

3. To get at terms with some peculiar quantum mechanical predictions that deal with the notion of *non-locality*, which, in Bell's words, "seem almost to cry out for a hidden variable interpretation [20]". These predictions have to do with the specific quantum mechanical correlations exhibiting *non-locality* that EPR[56] first addressed in their famous paper. The peculiarity of these correlations has to do with the fact that the correlations determined between two spatially distinct quantum systems *seem* to be determined in advance by certain dynamical variables at the time of the interaction that also correlated the systems after their separation. (As an example one could think of some dynamical variables that in the interaction must meet a certain conservation law.) If indeed these variables –hidden or not– correlate the systems, then the outcome of one measurement makes it possible to predict the outcome of the other without invoking some instantaneous action at a distance. The description could then be 'local'. However quantum mechanics does *not* specify these variables and one is left with the puzzling aspect of how to account for these peculiar, perhaps even non-local, correlations.

These three motivations to study hidden variables ask for a specific hidden variable formalism that embeds the quantum formalism. This formalism is often referred to as the doctrine of *local realism* (see also definition 4.2.3). Thus, the hidden variables program for quantum mechanics asks for a local realistic account of the quantum phenomena. The following question then arises naturally.

> Can one answer the incompleteness problem with local realistic hidden variables?

The first breakthrough in answering this question was the ground breaking paper by Einstein, Rosen and Podolski [56] in which they envisaged a *Gedankenexperiment* referred to as the EPR paradox[3]. We have already seen the EPR paper in the introduction of chapter 2 because in it the peculiar features of entangled states first appeared. However the real reason that EPR decided to use these states was to set up an argument against the completeness of quantum mechanics.

I will not go into the details of the EPR argument. Only the logical form of the *Gedankenexperiment* is here important. It goes as follows. If predictions of quantum mechanics (QM) are correct then there is a conflict between the two statements that the experimental results can be described in a local-realistic way and quantum mechanics provides a complete description of physical systems. The first view is called local realism (LR) the second completeness of quantum mechanics (CQM). The EPR paradox now can be shown in its symbolic form as [95]:

$$\text{QM predictions} \implies \neg\,(\text{LR} \wedge \text{CQM}). \tag{4.1}$$

[3]Much can be said about the EPR program and some say that that it was a plea for hidden variables. However, I will say only this: Einstein and his co-workers Podolski and Rosen contributed to the development of HV-theories. "But, as is not uncommon in the history of physics, the intellectual originator of a theory does not necessarily identify himself with the full-fledged development"[87]

EPR considered LR to be true so they concluded that if QM is correct then QM is incomplete.

However the second breakthrough in answering the hidden variables question was by John Bell in 1964 who showed that a stronger result can be obtained in which the option EPR chose –the incompleteness of QM– is no longer possible. Bell [16] proved this using the by now famous Bell-inequalities. He showed that if one accepts the predictions of QM then LR cannot hold. There is no need to invoke the completeness of QM. The logical form of the so called Bell-theorem is as follows:

$$\text{QM predictions} \quad \Longrightarrow \quad \neg\ \text{LR}. \tag{4.2}$$

Thus Bell proved that if quantum mechanics is correct local realism cannot hold. Bell has a stronger statement than EPR although both EPR and Bell use in essence the same two particle entangled quantum states. But Bell takes more measurements into account and can thus make a stronger statement. The consequence of Bell's 1964 work is that no local realistic hidden-variable theory can reproduce all the quantum mechanical experimental predictions. This brings the incompleteness problem into the experimental realm, and this is often referred to as a turn towards "experimental metaphysics", and indeed experimental tests of the Bell-theorem have been performed.

Bell's theorem is in essence a no-go proof against non-contextualist hidden variable theories. No-go proofs against non-contextualist hidden variable theories were given by von Neumann [19], Kochen and Specker [18] and Bell [16] himself. However Bell was the first to translate the requirement of non-contextuality into the physical assumption of locality and thereby into experimental terms. Consequently he opened the field towards experimental tests. Subsequently in later years many different Bell-theorems appeared depending upon what specific model they want to exclude. However all use a violation of a certain Bell-type inequality. Further, Bell-type theorems typically involve probabilistic, modal and spatiotemporal notions. The common feature of all Bell-type theorems is the deduction of an experimentally accessible prediction from a set of assumptions about the properties of the assumed hidden variables and this predictions is subsequently shown to be in conflict with a quantum mechanical prediction for the same system subjected to same set of measurements. The set of assumptions about the functioning of the hidden variables are motivated by quite general views such as locality, determinism, realism with respect to properties and freedom of the experimenters choices.

Because of the conflict with the quantum mechanical prediction and because of the overwhelming experimental evidence against the predictions of local hidden variable models, at least one of the assumptions is very likely not to be satisfied in the natural world. Finding out which of the assumptions must go and what this exactly implies for our world view is not what I here will pursue into. I will stay at an operational level and will refrain myself from speculation about metaphysical consequences of the refutation of Bell's inequality. I will mainly concern myself with technical questions like: What is the exact formulation of the various Bell-theorems? What are the most general constraints on correlations imposed by local realism? Which quantum states violate these constraints and what is the relationship between such a violation and other properties of the quantum mechanical state space (This is mainly treated in the next chapter)?

In the literature many different types of hidden variable models using different kinds of premises are used. I will use a very general and generic model: a stochastic hidden variable theory for orthodox quantum measurements. Later on in chapter 6 I will treat extended models for the more complex generalized quantum measurements. But before going into extensions first I will give the hidden variables formalism itself.

4.2 Bell-Theorem and Derivation of the Bell-Inequalities

4.2.1 Basic Notation and the Formalism of Hidden Variable Theories

In this section I present the formalism of hidden variable theories (HV-theories) as it has been used to answer the incompleteness problem, i.e. in the attempt to give an underlying explanation of the predictions of orthodox quantum mechanics. I will follow the approach of Ref. [47].

The formalism used to reconstruct quantum mechanics under the so called 'hidden variables program' is analogous to the reconstruction of thermodynamics by statistical physics. It comprises the following ingredients:

- **State space.** The state space Λ is used which is analogous to the state space Ω of the classical formalism used in appendix F. The pure states are represented by 'points' in the state space Λ and are denoted by λ, the so-called 'hidden variable'. The exact form of λ is not specified and is left unrestricted.

- **States.** A basic assumption of this program is that the system always is in one of the pure states $\lambda \in \Lambda$, even though this exact state might not be known. Furthermore, the state variable λ is supposed to determine all results of all possible measurements. A general mixed state is a normalised probability distribution $\mu(\lambda)$ on the phase space Λ of hidden variables λ, i.e. $\int_\Lambda \mu(\lambda) d\lambda = 1$.

- **Physical quantities.** For any given λ every physical observable $\mathcal{A}$ has a precise value notated as $A[\lambda]$ and which is revealed upon measurement. Thus any physical quantity $\mathcal{A}$ can be represented by a real-valued function on the space Λ in the following way: $A : \Lambda \to \mathbb{R}$. It is assumed that the values of $A[\lambda]$ are identical to the values found when measuring $\mathcal{A}$.

- **Quantum-criterium (Orthodox measurement) [47]:**

  A further requirement of the 'hidden variable program' is that every physical quantity represented by quantum mechanics must have a counterpart in the HV-theory. This means that the set of values of the real-valued function A has to be identical to the complete spectrum of the operator[4] $\hat{A}$ which corresponds according to quantum mechanics to the observable $\mathcal{A}$. Further

[4] In this section the self-adjoint operators acting on $\mathcal{H}$ will be denoted by $\hat{A}$ whereas ordinary real-valued functions on Λ by A.

the expectation value of $\mathcal{A}$ when the system is in the state μ_ρ which according to the HV-theory corresponds to the quantum mechanical state ρ, has to be identical to the quantum mechanical prediction for this expectation value:

$$E^{HV}_{\mu_\rho}(A) := \int_\Lambda A[\lambda]\mu_\rho(\lambda)d\lambda = Tr[\hat{A}\rho]. \tag{4.3}$$

Note that this criterium encapsulates the (extended) quantum postulates 1', 2', 3' and 4' of *orthodox* quantum mechanics (see section 2.2 and 2.5).

Thus, the 'hidden variables program' wants a hidden-variables theory for *for orthodox* quantum mechanics, i.e. the theory has to meet the Quantum criterium. This is the requirement that the HV-theory is in line with the quantum mechanical postulates 1', 2', 3' and 4'. If the desired HV-theory meets this criterium, then all possible quantum mechanical probabilities of the orthodox formalism (which are all given by $Tr[P\rho]$ with P in the set of projection operators $\mathcal{P}$) can be represented by their corresponding HV-probabilities simply by following the instructions of Eq.(4.3). In the next section we will see what constraints are implied by this Quantum-criterium for the construction of HV-theories and this will lead to a specification of further constraints that usually are required under the 'hidden variables program', such as the requirement of locality.

4.2.2 The Incompleteness-problem Revisited, Von Neumann's 'No-go Proof' and Bell's analysis

In this section I present a historical review about how the incompleteness problem –reformulated using the above mentioned Quantum-criterium for HV-theories– has led to the Bell-theorem and the Bell-inequality. The theorem and inequality themselves are treated in the next sections.

The incompleteness problem as defined in definition 4.1.1 is not a sharp mathematical problem and is rather ambiguous depending upon personal philosophical inclination about the idea of 'completeness'. However, the definition of a HV-theory underlying quantum mechanics as given in the last section, supplemented with the formulation of the Quantum-criterium, enables us to give a sharper formulation of the incompleteness problem:

Definition 4.2.1 (Incompleteness problem, sharper formulation). *Does a HV-theory exist which obeys the Quantum-criterium? [47].*

This is indeed the case. A very trivial example can be given which I call the *Toy HV-theory*. One just has to choose the space Λ of hidden variables big enough to be able to reproduce all possible measurement results and quantum mechanical predictions for the system under consideration. Suppose we have a certain collection of possible measurement results $\{a_i\}$, $\{b_j\}$, ... for measurement of a set of quantities $\mathcal{A}$, $\mathcal{B}$, ... of a certain system in the quantum state ρ.

For simplicity and clarity, first consider the case that the results and predictions of only one observable, let's say $\mathcal{A}$, has to be represented by the HV-model. Each result a_i of the possible set of measurement results of the quantity $\mathcal{A}$ (which according to quantum mechanics must be in the spectrum of the corresponding observable $\hat{A}$) is given an independent hidden variable λ_{a_i}. The hidden variable space $\Lambda \subset \mathbb{R}$ for this system now trivially consists of all points λ_{a_i}.

This can of course be extended to the case of more than one observable where one then gives each joint occurrence of two or more measurement outcomes for the measured observables a single hidden variable. E.g., the occurrence of the measurement outcome a_i and b_j after measurement of the quantities $\mathcal{A}$ and $\mathcal{B}$ on the same system is given the hidden variable λ_{a_i,b_j} such that $A[\lambda_{a_i,b_j}] = a_i$ and $B[\lambda_{a_i,b_j}] = b_j$. Every possible combination of measurement results is thus associated with a unique hidden variable and together they constitute the space Λ. If one wants to measure a new observable, then the hidden variables are changed accordingly to incorporate the possible measurement results of this new observable. To conclude we could say that in this Toy HV-model the hidden variables are nothing but all combinations of the possible measurement results of the set of observables themselves.

This model furthermore needs a probability measure $\mu(\lambda)$ with $\sum_{a_i,b_j,\ldots} \mu(\lambda_{a_i,b_j,\ldots}) = 1$, because the Quantum criterium requires that all predicted quantum mechanical expectation values for the possible measurements on this system in the state ρ can be reproduced by the HV-theory. In this Toy-model this measure (corresponding to the state ρ) is the trivial measure

$$\mu_\rho(\lambda_{a_i,b_j,\ldots}) := Tr[P_{a_i}\rho]Tr[P_{b_j}\rho]Tr[\ldots], \tag{4.4}$$

where P_{a_i} is the projection operator for the eigenvalue a_i of operator $\hat{A}$, etc. It is easy to check that this measure is in accordance with the requirement of Eq.(4.3); it reproduces all quantum mechanical probabilities (such as $Tr[P\rho]$ with $P \in \mathcal{P}$) and expectation values (such as $Tr[\hat{A}\rho]$) for the measurements on the system under consideration [47]. For example the expectation value of observable $\mathcal{A}$ in the HV-theory is given by

$$E^{HV}_{\mu_\rho}(A) := \int_\Lambda A[\lambda]\mu_\rho(\lambda)d\lambda = \sum_{i,j,\ldots} A[\lambda_{a_i,b_j,\ldots}]\mu_\rho(\lambda_{a_i,b_j,\ldots}) = \sum_i a_i Tr[P_{a_i}\rho], \tag{4.5}$$

which indeed is in accordance with the quantum mechanical prediction.

Given that in general there is no limit to the number of observables and thus neither to the number of possible quantum mechanical predictions, the above used assignment of hidden variables implies that one has to use an *infinite* amount of hidden variables to completely describe the system in the HV-theory.

Although this Toy HV-theory is mathematically possible it has no physical significance whatsoever since it uses an *ad hoc* assignment of an infinite number of hidden variables and furthermore does not incorporate the essential idea that physical laws and specific relations exist between certain observables. It treats all observables as statistically independent which is not in accordance with the picture of the physical world which physics gives us [47]. Indeed, in this picture, some observables are functions of other observables or give a certain relation between other observables.

This Toy HV-model shows us that in order for the HV-theory to be physically acceptable other constraints than just the Quantum-criterium have to be demanded of the theory as well. This has the important conclusion that in the incompleteness problem as stated above we should ask not just for *any* HV-theory meeting the Quantum-criterium but for *physically acceptable* HV-theories. Accordingly, the definition of the incompleteness problem has to be changed to the following final version:

Definition 4.2.2 (Incompleteness problem, final version). *Does a physically acceptable HV-theory exist which obeys the Quantum-criterium?*

Although this definition is more restrictive than the previous one, it is also more ambiguous since the question of which constraints one has to demand to get a physically acceptable HV-theory has been the topic of long and everlasting debate. For example, in the very first proof of the negative answer to the incompleteness problem, which is due to Von Neumann [19], certain algebraic relations which hold between quantum mechanical quantities are also postulated to hold between the corresponding quantities of the HV-theory. These are treated in detail below in Eq.(4.7). These relations seem to be very plausible at first sight. However, Von Neumann showed in his famous theorem that no HV-theory that satisfies the Quantum-criterium can also satisfy these relations. For many decades this 'no-go proof' (of the existence of any HV-theory for quantum mechanics) of the well-respected Von Neumann was taken for granted and most physicists therefore believed that no other theory besides quantum mechanics could exists that would explain the micro physical observations. It was believed that the incompleteness problem had been solved by Von Neumann and that the answer was definitely negative. Consequently, concern over incompleteness of QM vanished almost completely and for decades this problem was only addressed by a few who were ignored by the physics community.

However, it was slowly realized through the contribution of many authors that von Neumann's theorem could really rule out only special classes of HV-theories: those that satisfy its assumptions[25]. And in 1964 John Bell showed that the widespread belief that Von Neumann had proven the impossibility of any reasonable HV-theory was in fact preliminary. Bell reopened the discussion of hidden variables in the first of his great papers [16] (written in 1964 but only published in 1966) by giving a careful analysis of Von Neumann's famous proof and its axioms.

He demonstrated that von Neumann's argument unreasonably assumed that *all* hidden variables must fall in line with the rules obeyed by the usual quantum mechanical variables. It is the case that the usual quantum mechanical variables expectation values are linear, i.e. for all possible states ρ they obey the equation:

$$\mathrm{Tr}[(\alpha\hat{\mathrm{A}}+\beta\hat{\mathrm{B}})\rho]=\alpha\mathrm{Tr}[\hat{\mathrm{A}}\rho]+\beta\mathrm{Tr}[\hat{\mathrm{B}}\rho]. \tag{4.6}$$

Von Neumann now required that the same linearity holds for *all* hidden-variable states, and in particular for the pure hidden-variable-states; i.e. the following must hold for all $\lambda\in\Lambda$

$$(\alpha A+\beta B)[\lambda]=\alpha A[\lambda]+\beta B[\lambda]. \tag{4.7}$$

Because the values of $A[\lambda]$ are the eigenvalues of the corresponding operators one can easily see that in general this requirement can not be met.[5] Therefore

[5]For example, let us look at the example Bell gave [16]. Consider the non-commuting spin observables σ_z and σ_x for a spin $\frac{1}{2}-$particle. The eigenvalues for both operators are ±1 whereas for the operator $\sigma_z+\sigma_x$ the eigenvalues are $\pm\sqrt{2}$.

Von Neumann concluded that it is impossible for any HV-theory to meet the Quantum-criterium.

However, Bell argued in his article that this requirement of Eq.(4.7) is physically unreasonable. According to him there is no *a priori* commitment for the hidden variables to obey Eq.(4.7) because different experiments are required to perform the measurements of the observables corresponding to $A+B$ and to A and B individually. So there is no a-priori reason to suppose that an algebraic relation exists between these different measurements. The validity of the relationship of Eq.(4.6) for pure states and for all possible sets of observables A and B (commuting and non-commuting) has to be considered as a special feature of QM and not as a universal feature for all possible theories [47].

Bell had been greatly influenced by Bohm's hidden variable model of 1952 also well-known as 'the Bohm-mechanics' or 'pilot-wave theory'. He wrote about this: "In 1952 I saw the impossible done." ([20], p.160). Indeed, according to Von Neumann's proof the impossible had been done. Bohm had constructed a theory using the so-called 'quantum potential' that reproduced all quantum mechanical predictions and which was at the same time in accordance with the above mentioned requirements far a hidden variable theory. In other words, Bohm had constructed a hidden variable theory that did meet the Quantum-criterium, and thereby answered the incompleteness problem to the positive.

Von Neumann's proof was correct, yet Bohm had provided a counterexample to its conclusion. What then was the problem with this proof? Bell showed in his article that Bohm's HV-theory just does not meet the assumptions of von Neumann's proof, i.e., it does not meet the requirement of Eq.(4.7) which Von Neumann used in his 'No-go theorem'.

This analysis of Bell showed that Von Neumann's' requirement of Eq.(4.7) for any HV-theory is unreasonable strong and that upon removal of this requirement the proof 'collapses' and the incompleteness problem is again left unanswered. In order to get an answer we have to ask the following: What other, physically reasonable, requirements can be asked of a HV-theory to get a satisfactory answer to the incompleteness problem? Does perhaps Bohm's HV-theory provide such a theory?

Before answering this question I will first discuss an important theorem which has to be kept in mind when trying to find reasonable premises for the construction of any HV-theory. The linearity requirement of Eq.(4.7) used by Von Neumann for commuting observables is a special case of the general assumption that functional relations among commuting) quantum operators represent functional relations among the corresponding HV-observables. Suppose that $\hat{B} = f(\hat{A})$ then this assumption entails that $B[\lambda] = f(A[\lambda])$, i.e.

$$f(A)[\lambda] = f(A[\lambda]). \tag{4.8}$$

This *Func-rule* (Eq.(4.8)) implies the so-called Sum-rule of Eq.(4.7) used by Von Neumann, but only for the case of commuting observables. This requirement of the Func-rule, which could be defended as a reasonable requirement for any HV-theory, nevertheless inhibits the possibility of a HV-theory for quantum mechanics. This is the remarkable content of the theorem of Kochen en Specker:

Theorem 4.2.1 (Kochen-Specker). *No value-assignment (which is in accordance with the HV-theory postulates) exists for systems with a Hilbert space of dimension $N > 2$ that is able to reproduce for all observables the Func-rule of Eq.(4.8). In other words, a contradiction exists between the postulates of the HV-theories supplemented with the requirement of Eq.(4.8) and the postulates 1', 2' and 3' of quantum mechanics. Note that the Born-postulate, postulate 4', is not needed. For proof of this theorem see [18].*

On the one hand, the requirement to reproduce *all* functional relationships in accordance with Eq.(4.8) leads to the impossibility of any HV-theory that meets postulates 1' to 3' of quantum mechanics and thus by implication also to the impossibility of any HV-theory that meets the Quantum criterium. However, as we have seen Bell has shown in his analysis of Von Neumann's 'no-go' proof that this is too strong a requirement.

On the other hand, to require *no* functional relations *whatsoever*, as in the above mentioned Toy HV-theory, does allow for the construction of a HV-theory that meets the Quantum-criterium. However, we have seen that this theory is physically meaningless.

Then, what sort of functional relationships *can* we ask of our HV-theory which *are* physically reasonable so that the theory is physically meaningful while *at the same time* demanding that the theory is in accordance with the Quantum-criterium?

To investigate this question, let's lets go back to the Toy HV-theory and try to understand why this theory is able to reproduce all measurement results of a set of measurements for a specific system under consideration. Why does the Toy HV-theory work? Because some form of *contextuality* is used in the assignment of the hidden variables. I will try to explain this in what follows. I will only give a restrictive account of contextuality suitable for the purposes needed here, but note that idea of contextuality is far more general.

The Toy HV-theory is one of the simplest HV structures from which all measured results can be obtained: the set of hidden variables are either the *actual* collection of measured data itself or the *actual and possible* collection of data for the specific set of observables to be measured. For example, the hidden variables $\lambda_{a_i,b_i,...}$ of the Toy model depend upon the outcomes $a_i, b_i, \ldots$, and therefore upon the measuring devices (represented by the HV-observables $A, B, ..$) chosen by all the parties. This feature marks the so called *contextual* hidden variable theories; the hidden variables depend upon the specific experimental context (such as the particular observables and outcomes of measurement) and not merely on the state specification of the system prior to measurement.

However, this sort of contextuality is unreasonable and far too blatant. Why? Because this extreme form of contextuality (i.e. dependency of the hidden variables upon the outcomes themselves) implies that the theory has no great predictive power; all future unspecified measurements are hidden and no predictions for them can be given whatsoever. Furthermore this contextuality rules out all physical laws or meaningful relationships between observables. The context it requires is too greatly and therefore restrictively specified for this.

Nevertheless, the idea that the context of measurement has to be incorporated in the theoretical formalism of HV-theories is not all that stupid. It was mentioned by Bell in his article that analyses Von Neumann's 'no-go' proof. Bell thought this idea of contextuality to be in line with Bohrs requirement of the specification of what actually constitutes a quantum phenomenon[6]. In this article he gives some remarks about what sort of demands one is allowed to ask of a *contextual* HV-theory to obey; In other words, Bell's concern was about what reasonable assumptions concerning contextual relations one *can* ask from a HV-theory.

According to Bell, these assumptions have to have a spatial meaning and must allow for a space-time vision of the evolution of any system from preparation to measurement, i.e. the contextual specification must be local and allow for a space-time picture of the dynamics.

This idea of contextuality in a spatial context was used long before Bell thought of it. Not only EPR used it in their famous article but also Bohm in the construction of his HV-theory. Bell was the first to notice this when he asked himself: Why did Bohm's HV-model actually work? What made it get out of the reach of Von Neumann's 'no-go' theorem and why did it not violate the Kochen-Specker theorem? Bell showed that Bohm's model did allow *certain* functional relations among the HV-observables (which made the theory physically interesting) which had a contextual nature so that the Kochen-Specker theorem was not violated. But Bell noticed in his paper that these contextual relations in Bohm's theory are grossly *non-local*, i.e. Bohm mechanics is actually a non-local HV-theory. The contextual formulation of the dynamics allows for non-local characteristics. At the conclusion of his paper, Bell surmised that *all* hidden variable theories might have this property of non-locality and suggested that those interested should look for a proof of this hypothesis.

Quite soon Bell came up with a proof of his own which was based on the EPR paper. In this second paper of Bell (published in 1964 but written after his first paper which was only published in 1966), he showed that all deterministic HV-theories that obey the QM-criterium have to be non-local (or contextual, since non-locality is a sufficient condition for contextuality). In this proof he used his by now famous inequalities, the so-called *Bell-inequalities*. With the tentative acceptance of quantum mechanics and of locality, the conclusion was that deterministic hidden variables were not possible. Later on however, the requirement of determinism was relaxed while maintaining the same argument. Bell thus proved that all local HV-theories, also called *classical* or *local realistic theories*, cannot be in accordance with the Quantum-criterium. This is the so-called *Bell-theorem*.

Having finally arrived at the Bell-theorem, this ends the historical story of the emergence of the Bell-theorem from the incompleteness problem. But the physical and mathematical story has just begun; for it is the case that the above mentioned formulation of the Bell-theorem uses the *ambiguous* notions of non-locality and of the related doctrine of local realism. But what actually is meant by them? In the next section these concepts will be defined. This leads to the Bell-inequality and a more strict formulation of Bell's theorem will subsequently

[6] According to Niels Bohr, every *quantum phenomenon* is the totality of the preparation device, measurement device, the specific physical system and their mutual interactions in a concrete experimental setup [47].

be given.

4.2.3 Constraints on Correlations: Local Realism

In section 4.2.1 the mathematical formalism of any HV-theory has been given. In the last section we have seen that one has to ask certain specific requirements of the HV-theory for it to be physically meaningful, although the form of the exact requirements themselves was still left an open question. The requirements of Von Neumann were rejected by Bell. He himself then started the (everlasting) search for what requirements were physically reasonable if one wanted to complete quantum mechanics by constructing a HV-theory for all its predictions. One set of these requirements –which Bell investigated himself– is given by the so-called doctrine of local realism. This doctrine leads to the local hidden variable theories which are supposed to present the fundamental structure of classical physics. This research has led to the Bell-inequalities for HV-theories which are constraints on correlations arising from this doctrine of local realism.

In the next two sections these Bell-inequalities and the doctrine of local realism will be strictly mathematically presented in a setting which easily allows for the formulation of the Bell-theorem, which is subsequently presented in the following section. I will follow the approach of [58].

Bell-inequalities are always formulated in terms of *correlations* between two or more spatially separated observers. Each of the observers gets a particle (i.e. subsystem) from a common source, which is subjected to a specific measurement procedure. See figure 4.1.

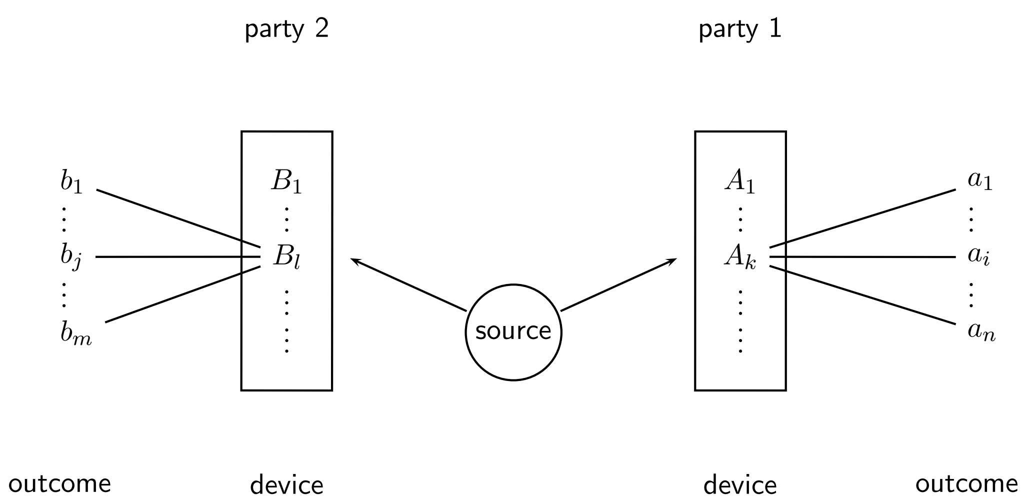


Figure 4.1: General bi-partite setup.

The correlations between the measurement outcomes of the different parties are the joint probabilities to get a certain joint measurement result. These measured probabilities for the bi-partite case are denoted by

$$\mathbb{P}(a_i, b_j | A_k, B_l), \tag{4.9}$$

where a_i and b_j are the possible outcomes for measurement of the devices A_k and B_l used respectively by parties 1 and 2. Only finitely many outcomes are possible for each measurement. The collection of all these probabilities of Eq.(4.9), called the *correlation table* [58], are the data which any HV-model has to reproduce.

The data of this correlation table have to satisfy some constraints. Some of them follow already from the probability interpretation of the numbers of Eq.(4.9). All probabilities are positive and for a particular setup (A, B) they have to add up to unity:

$$\mathbb{P}(a_i, b_j|A_k, B_l) \geq 0 \qquad \sum_{a_i, b_j} \mathbb{P}(a_i, b_j|A, B) = 1. \tag{4.10}$$

The probabilities measured by only one party are the *marginals* and in the exemplary case of observer 1 these are denoted by:

$$\mathbb{P}(a_i|A, B) = \sum_{b_j} \mathbb{P}(a_i, b_j|A, B). \tag{4.11}$$

For general systems it is possible that the correlation tables give rise to marginals that depend on the whole setup. Thus in general the marginals for party 1 can depend on the device B chosen by party 2.

Apart from the obvious constraints arising from the probability interpretation of the numbers of Eq.(4.9) other constraints are formulated based on certain physical arguments. Before presenting the constraints leading to Bell inequalities I have to formalize both the doctrine of local realism, which gives rise to these constraints and the corresponding idea of a local HV-theory for correlation tables. This is accomplished by explicitly introducing a hidden variable λ in a space Λ. Assume that the systems sent to party 1 and 2 are described by λ in sufficient detail so as to compute the probabilities of the response to any measurement. This is the most general situation where only the probabilities of the results to occur are determined and not the results themselves; i.e. the hidden variables are *stochastic* and not per se deterministic.[7] This means that for any measuring device A of party 1 and B of party 2 and any possible joint measurement outcome a and b of these respective devices, a *response probability function* $p_{A,B}(a, b, \lambda)$ is obtained [58]. Further, the source of the correlation experiment is characterised by a probability measure $M(\lambda)$ on Λ which gives the probabilities with which each λ occurs. With this specification all correlations of Eq.(4.9) can now be computed in this HV-model as follows:

$$\mathbb{P}(a, b|A, B) = \int d\lambda \; p_{A,B}(a, b, \lambda). \tag{4.12}$$

This response probability function $p_{A,B}(a, b, \lambda)$ can always be written in terms of the conditional probabilities in the following way:

$$p_{A,B}(a, b, \lambda) = p_{A,B}(a \;|b, \lambda) \; p_{A,B}(b \;|\lambda) \; M_{A,B}(\lambda). \tag{4.13}$$

The doctrine of local realism leading to the Bell-inequalities will now be defined using the following three assumptions on the conditional probabilities of

[7] See footnote 8 for a discussion of the relationship between deterministic and stochastic HV-theories.

Eq.(4.13). I will use the formulation of [47] although these assumptions were first distinguished by Jarrett[15].

1. Outcome independence. The probability to obtain a result a for the observable A is completely determined by the experimental setup (i.e the measurement devices A and B) and the hidden variable λ. There is no dependency on the result b.

$$p_{A,B}(a\,|b,\lambda) = p_{A,B}(a\,|\lambda) \quad \text{and} \quad p_{A,B}(b\,|a,\lambda) = p_{A,B}(b\,|\lambda). \tag{4.14}$$

2. Parameter independence. The probability to obtain a result is only locally determined, i.e. it is independent of the distant measurement device:

$$p_{A,B}(a\,|\lambda) = p_A(a\,|\lambda) \quad \text{and} \quad p_{A,B}(b\,|\lambda) = p_B(b\,|\lambda). \tag{4.15}$$

3. Independence of the source. The hidden variable distribution of the source is independent of the particularly chosen measurement setup:

$$M_{A,B}(\lambda) = M(\lambda). \tag{4.16}$$

The conjunction of these three conditions leads to the following expression for the probability response function:

$$p_{A,B}(a,b,\lambda) = p_A(a|\lambda)p_B(b|\lambda)M(\lambda). \tag{4.17}$$

From this it follows that

$$p_{A,B}(a,b|\lambda) = p_A(a|\lambda)p_B(b|\lambda). \tag{4.18}$$

This result states the outcomes a and b for a fixed λ are completely statistically independent. This is often called *factorisability* [47].

Using this factorisability the correlations of the correlation table will be given by:

$$\mathbb{P}^{\text{lr}}(a,b|A,B) = \int d\lambda p_A(a|\lambda)p_B(b|\lambda)M(\lambda). \tag{4.19}$$

A correlation table is said to allow a *local HV-model* or a *classical* or a *local realistic* (lr) *model* if all correlations can be represented as in Eq.(4.19)[8]. Such correlations are often referred to as being *classically correlated*. Conversely, *non-classical* and *non-local* correlations are correlations that cannot be modeled in this form.

This definition of a local HV-model allows me to finally define the doctrine of local realism which is supposed to present a fundamental physical feature of all classical physics:

[8]Note that in the above defined local HV-model only the probabilities to obtain certain results are determined by the hidden variables and not the results themselves. Therefore these HV models are also called *stochastic* local HV-models in contrast to *deterministic* local HV-models (where the results themselves are determined by the hidden variables). In these deterministic HV-models the response probability functions take only the values 0 and 1. However, this seemingly stronger constraint of deterministic response functions does not lead to sharper constraints on the correlation data. The reason is that every stochastic HV-theory can be upgraded to a deterministic one by adding additional variables, see for instance [58].

Definition 4.2.3 (Local realism). *All correlations in correlation tables for all physical systems obtained from actual or possible physical measurements allow a local HV-model. In other words, factorisability as given in Eq.(4.18) of all response probabilities for all correlation tables of all physical systems holds.*

For those familiar with issue of contextuality in hidden variable theories, note that local realism is the doctrine of a specific sort of contextual hidden variables where the contextuality is actually physically constrained to local contexts motivated through the idea of locality.

4.2.4 The Bell-Inequality

In this section I will show that the above formulated constraints that imply factorisability of the response probability functions and which make up the doctrine of local realism, lead to the so-called *Bell-inequalities*. These inequalities present sufficient conditions and in some cases even necessary[9] conditions for the existence of a local HV-model for a certain correlation table and thus for the validity of the doctrine of local realism.

The standard example of the Bell inequality is the Clauser-Horne-Shimony-Holt (CHSH) inequality for the EPR experiment in the version as presented by Bohm [2] (also called the EPRB-experiment). In this setup there are correlation measurements on two spin-$\frac{1}{2}$ particles prepared at a single source characterised by the hidden variable distribution $M(\lambda)$. The particles are then spatially separated and the spin on each particle is measured in a certain direction by measuring devices A and B. In other words, two dichotomic (± 1-valued) observables A and B are measured on two different spatially separated sites. See figure 4.2.

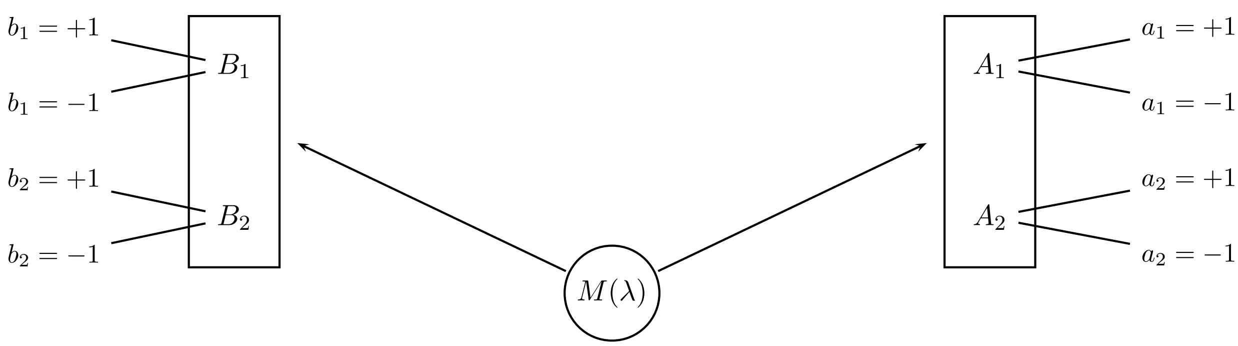


Figure 4.2: Setup for EPRB experiment.

Let us now assume that local realism holds for the possible correlations of the correlation table in this experiment. Factorisability is thus assumed, i.e. the response probability functions for measurements on each of the spatially separated sites are thus given by respectively $p_A(a|\lambda)$ and $p_B(b|\lambda)$ with $a = \pm 1, b = \pm 1$.

[9]See section 4.4.1 for a discussion of sufficient *and* necessary conditions for local realism.

This represents the assumption that the responses on each site are taken to be statistically independent. Let us now consider the mean value for the random variable a and b in terms of the response probability functions:

$$\bar{a}(\lambda) = p_A(+1,\lambda) - p_A(-1,\lambda) \quad \text{and} \quad \bar{b}(\lambda) = p_B(+1,\lambda) - p_B(-1,\lambda). \tag{4.20}$$

It follows that $|\bar{a}(\lambda)| \leq 1$ and $|\bar{b}(\lambda)| \leq 1$. From these mean values the so-called correlation function $\mathcal{B}$ is constructed as follows:

$$\mathcal{B}(\lambda) = \frac{1}{2}\left[\bar{a}_1(\lambda)(\bar{b}_1(\lambda) + \bar{b}_2(\lambda)) + \bar{a}_2(\lambda)(\bar{b}_1(\lambda) - \bar{b}_2(\lambda))\right], \tag{4.21}$$

where $\bar{a}_1$ and $\bar{a}_2$ refer to two different measurements performed by measurement devices A_1 and A_2 (and similarly for $\bar{b}_1$ and $\bar{b}_2$).

The CHSH inequality now arises from the fact that the correlation function $\mathcal{B}$ satisfies the pointwise inequality $|\mathcal{B}| \leq 1$. This follows from the fact that $|\bar{a}(\lambda)|$ and $|\bar{b}(\lambda)|$ are bounded by unity.

The expectation value of $\mathcal{B}$ is the so-called *Bell correlation* τ:

$$\tau = \int M(\lambda)\mathcal{B}(\lambda)d\lambda. \tag{4.22}$$

It is also bounded by unity because $\mathcal{B}(\lambda)$ is pointwise bounded. Using the expectation values $E(A,B) = \sum_{a,b=\pm1} a\, b\, \mathbb{P}(a,b|A,B)$ this Bell correlation τ can be expressed directly in terms of the measurable quantities of the correlation table., i.e the inequality $|\tau| \leq 1$ the becomes the famous *CHSH inequality* [24]:

$$\left|E^{\text{lr}}(A_1,B_1) + E^{\text{lr}}(A_2,B_1) + E^{\text{lr}}(A_1,B_2) - E^{\text{lr}}(A_2,B_2)\right| \leq 2. \tag{4.23}$$

This CHSH inequality is a necessary condition for factorisability of all response probabilities of the correlation table of this experiment. In other words, if the data in the correlation table of this experimental setup meet the CHSH-inequality, then a local hidden variable model for this data is possible and one could say that local realism holds for this part of the physical world. Conversely, if the CHSH inequality is violated, then no local hidden variable model is possible and in accordance with definition 4.2.3 the data is said to be non-local.

4.2.5 The Bell-Theorem

Let's go back to the final version of the incompleteness problem as defined in section 4.2.2: Does a physically acceptable HV-theory exist which obeys the Quantum-criterium? We have seen that in order to answer this question a specification is needed of what it means for a theory to be physically acceptable. Without giving further elaborations at this moment a lot of physicists thought there to be good reasons to demand that any physical theory has to be (at least) in accordance to local realism, i.e. all correlation tables in this theory have to have a local HV-model and thus all probabilities in the EPRB experiment have to obey the CHSH-inequalities. However, Bell has proven that this cannot be the case when one wants the physical theory to be in accordance to the Quantum-criterium. This is the content of the so-called Bell-theorem [47]:

Definition 4.2.4 (Bell-theorem). *A local HV-theory is empirically at odds with the Quantum-criterium, i.e. quantum mechanical predictions exist that violate the empirically accessible CHSH inequality.*

In order to proof this theorem we have to re-express the CHSH-inequality in terms of operators on a Hilbert space. The expectation values $E(A, B)$ are replaced by their quantum mechanical equivalents $E(\hat{A}, \hat{B}) = \mathrm{Tr}[\hat{A} \otimes \hat{B}\rho]$ for a system in a state ρ. Further the hidden variable λ is supposed to be the quantum state ρ, i.e. $M(\lambda) = \delta(\lambda - \lambda_0)$ with $\lambda_0 = \rho$. The Bell-inequality using these quantum mechanical measurements then becomes

$$|\mathrm{Tr}[\hat{\mathcal{B}}\rho]| = |\mathrm{Tr}[(\hat{A} \otimes \hat{B} + \hat{A}' \otimes \hat{B} + \hat{A} \otimes \hat{B}' - \hat{A}' \otimes \hat{B}')\rho]| \leq 2. \tag{4.24}$$

Now, recall figure 4.2. This experiment refers to correlation measurements on two spin-$\frac{1}{2}$ particles prepared at a single source in the so-called singlet state. This state is given on the direct product space $\mathbb{C}^2 \otimes \mathbb{C}^2$ as follows:

$$|\,\psi\rangle = 1/\sqrt{2}(|\uparrow\rangle\,|\downarrow\rangle - |\downarrow\rangle\,|\uparrow\rangle), \tag{4.25}$$

where $|\downarrow\rangle$ and $|\uparrow\rangle$ are the eigenstates with eigenvalues ± 1 of the spin or polarisation observable σ in a certain direction $\mathbf{n}$. The state $|\,\psi\rangle$ has total spin of zero and is therefore an eigenstate of the observable $\sigma \cdot \mathbf{n} \otimes \sigma \cdot \mathbf{n}$ with eigenvalue 0 for arbitrary direction $\mathbf{n}$. This singlet state is thus *rotationally symmetric.*

The spin correlation function of the singlet state as predicted by quantum mechanics is defined as $E_{QM}(\mathbf{a}, \mathbf{b}) := \langle\,\psi|\,\sigma_\mathbf{1} \cdot \mathbf{a} \otimes \sigma_\mathbf{2} \cdot \mathbf{b}\,|\,\psi\rangle$ with $\mathbf{a}, \mathbf{b}$ unit vectors in $\mathbb{R}^3$. Using the singlet state we find that $E_{QM}(\mathbf{a}, \mathbf{b}) = -\mathbf{cos}\ \theta_{\mathbf{a},\mathbf{b}}$. Inserting these expectation values into the CHSH inequality of Eq.(4.23) gives the following result:

$$\begin{aligned} |E_{QM}(\mathbf{a_1}, \mathbf{b_1}) + E_{QM}(\mathbf{a_2}, \mathbf{b_1}) + E_{QM}(\mathbf{a_1}, \mathbf{b_2}) - E_{QM}(\mathbf{a_2}, \mathbf{b_2})| &= \\ |-cos\ \theta_{\mathbf{a_1},\mathbf{b_1}} - cos\ \theta_{\mathbf{a_1},\mathbf{b_2}} - cos\ \theta_{\mathbf{a_2},\mathbf{b_1}} + cos\ \theta_{\mathbf{a_2},\mathbf{b_2}}| &\leq 2. \end{aligned} \tag{4.26}$$

If all correlations arising from the singlet state obey local realism then a local HV-model can be constructed and this inequality will hold. However, this inequality can be violated for a large set of measurement directions $\mathbf{a_1}, \mathbf{a_2}, \mathbf{b_1}$ and $\mathbf{b_2}$. For example, let us restrict our attention to the special case in which the four vectors are in one plane and (i) $\mathbf{a}$ and $\mathbf{b}$ are parallel, and (ii) $\theta_{\mathbf{a}',\mathbf{b}} = \theta_{\mathbf{a},\mathbf{b}'} = \phi$. Then the CHSH inequality will be satisfied provided

$$|1 - \cos 2\phi + 2\cos\phi| \leq 2. \tag{4.27}$$

However, as can be seen by plotting this function of ϕ, the inequality is violated for all values of ϕ between 0 and $\pi/4$. The largest violation is given by a value of $2\sqrt{2}$ which is the so-called Cirelson-bound [17]. It is proven in section 5.2.1.

We see that a specific state of two spin-$\frac{1}{2}$ particles exists, i.e the singlet-state of Eq.(4.25), such that measurements on the composed system give correlations for specific spin-directions that violate the CHSH-inequality. Because the CHSH inequality is a necessary condition for a local HV-model to exist, violation of this inequality is sufficient to conclude that no local HV-model for the correlations is possible. Finally, all these correlations given by $E_{QM}(\mathbf{a}, \mathbf{b})$ are empirically accessible[10]. This completes the proof of the Bell-theorem. Physical states that produce predictions that violate the CHSH inequality, such as the bi-partite singlet state used in the above argument, are called *Bell correlated* states. In chapter 5 I will investigate the properties of these Bell correlated states to see if the singlet state is the only one maximally violating the CHSH inequality.

An interesting fact that will be used later on in section 4.3 is that one cannot get a violation of the Bell-inequality if for all measurements one measures both particles in the same direction, i.e. if $\theta_{\mathbf{a},\mathbf{b}} = 0$ or π (and the same for $\theta_{\mathbf{a}',\mathbf{b}'}$). This means that no violation can be found for the cases in which measurement on one particle allows one to predict what happens to the other particle with absolute certainty, i.e. with probability equal to 1. For this is only the case where one measures the spin of one particle, and then measures the other either in the same or in the opposite direction. Not only does this case yield definite predictions by quantum mechanics, but in fact a local realistic model exist for these type of measurements, as Bell himself has shown [60]. Using the two-particle singlet state it is only in the case of an arbitrary angle between the measurements of the particles, where one does not have certain predictions, that quantum mechanics yields results that violate local realism.

Because the Bell-inequalities are violated in quantum mechanics one or more assumptions leading to these inequalities must be violated. Let us look at these assumptions of (i) outcome independence, (ii) parameter independence and (iii) independence of the source, as given in Eqs. (4.14), (4.15) and (4.16), and ask which of them will be violated.

Because the quantum states ρ are specified independently of the measurement setup, independence of the source as given in Eq.(4.16) holds. Furthermore, parameter independence holds as well. This is the content of the so-called *no-signaling theorem* (see for example Ref. [46]). In the above used spin example with ρ the singlet state, this can be seen by noting that the marginal probabilities to obtain any result are independent from any other measurement setup. In other words, $p_{\mathbf{a}}(a\,|\lambda) = Tr[\hat{A} \otimes \mathbb{1}\rho]$ and $p_{\mathbf{b}}(b\,|\lambda) = Tr[\mathbb{1} \otimes \hat{B}\rho]$ are both 1/2, where a and b are the possible results ± 1 of measuring the operators $\hat{A} = \sigma \cdot \mathbf{a}$, $\hat{B} = \sigma \cdot \mathbf{b}$. Lastly, does outcome independence hold in quantum mechanics? No, this is not the case. The probabilities $p_{\mathbf{a},\mathbf{b}}(a\,|b, \lambda)$ and $p_{\mathbf{a},\mathbf{b}}(b\,|a, \lambda)$ are not equal to $p_{\mathbf{a},\mathbf{b}}(a\,|\lambda)$ and $p_{\mathbf{a},\mathbf{b}}(b\,|\lambda)$ respectively. In our spin example this can be seen as follows. $p_{\mathbf{a},\mathbf{b}}(a = 1|\rho) = \frac{1}{2}$ while $p_{\mathbf{a},\mathbf{b}}(a = 1|b = 1, \rho) = \sin^2(\frac{1}{2}\theta_{\mathbf{a},\mathbf{b}})$. That quantum mechanics violates outcome independence is one of the remarkable features that has generated much philosophical debate. However, as noted before, I will not comment on this.

4.2.6 Bell-inequality as a Sufficient Condition for Entanglement

The quantum state of Eq.(4.25) which violates the Bell-inequality –the singlet state– is an entangled state. This is no coincidence because only entangled states

[10] In fact, the CHSH inequality has been experimentally tested on several occasions using both photons and atoms as the spin $\frac{1}{2}$- particles. The overwhelming result of these experiments is that the quantum mechanical predictions for violation of the CHSH-inequality are correct (although some loophole problems still remain).

can violate the Bell-inequality. In other words, the Bell inequality is a sufficient condition for bi-partite entanglement. This will now be shown.

Consider a state in which the two parties are independent from each other, i.e.: $\rho = \rho_1 \otimes \rho_2$. Then the Bell-inequality of Eq.(4.24) becomes

$$
\begin{aligned}
&|E_\rho(\hat{\mathcal{B}})| \\
&\quad = |\mathrm{Tr}[((\hat{A} + \hat{A}') \otimes \hat{B} + (\hat{A} - \hat{A}') \otimes \hat{B}')\rho] \\
&\quad = |(\langle\hat{A}\rangle + \langle\hat{A}'\rangle)\langle\hat{B}\rangle + (\langle\hat{A}\rangle - \langle\hat{A}'\rangle)\langle\hat{B}'\rangle| \\
&\quad \leq |\langle\hat{A}\rangle + \langle\hat{A}'\rangle| + |\langle\hat{A}\rangle - \langle\hat{A}'\rangle| \\
&\quad = 2\max(|\langle\hat{A}\rangle|, |\langle\hat{A}'\rangle|) \leq 2,
\end{aligned}
\tag{4.28}
$$

where I have used that $|\langle\hat{A}\rangle| \leq 1$ and similarly for $\hat{A}', \hat{B}$ and $\hat{B}'$.

Since $E_\rho(\hat{\mathcal{B}})$ is convex as a function of ρ this bound holds also for mixtures of the states considered, i.e. for all separable states. Hence for every non-entangled state we find:

$$|E_\rho(\hat{\mathcal{B}})| \leq 2. \tag{4.29}$$

Thus, a sufficient condition for bi-partite entanglement is a violation of (4.29).

4.3 More Complex Systems: Bell-Theorems without Inequalities and Algebraic Proofs

In 1989 an article appeared in a conference proceeding with the promising title 'Going beyond Bell's theorem'[27]. Many different versions of the Bell-theorem had already appeared of which most of them turned out to be of little relevance because they were nothing but 'variations on the same theme'. However this article was not just another one of those 'variations'. It turned out to contain some surprisingly new results that generated much debate.

Actually the article I am here talking about is the original article by Greenberger, Horne and Zeilinger which first used the by now famous GHZ-states. In it they come up with an algebraic proof of the impossibility of a local HV theory for quantum mechanics. In their own words: "Thus we reach the general conclusion that not only is there no way to form a classical local theory that reproduces quantum theory in general, but that even in the simpler case where one can make definite predictions in the EPR [local realistic] sense, it is impossible to do so with such a model." This proof is logically stronger than the original Bell-theorem. Greenberger, Horne and Zeilinger, together with Shimony, noticed this themselves in a paper called 'Bell's theorem without inequalities'[28].

This so-called GHZ-theorem attracted wide attention as a specific form of a Bell theorem without inequalities, the so called algebraic Bell-theorem. Again some variations on this same theme appeared. However in 1992 Hardy[34] published a new and different (logically weaker) version of a Bell-theorem without inequalities, the so-called Hardy theorem. According to Mermin, Hardy's theorem is the 'best version of Bell's theorem' [39] because it is "by far the simplest and cleanest case". This Hardy theorem differs from both the original Bell-theorem and from the GHZ-theorem in a fundamental way. However, both the GHZ-theorem and the Hardy-theorem use a more complicated quantum state and show that a certain logical (i.e. local realistic) reasoning breaks down when confronted with certain aspects of quantum mechanics which are notoriously different from the aspects used in the original Bell-theorem. In this sense they both go beyond Bell's theorem.

In this section I will analyse both these theorems and comment on the claim that they improve upon the Bell-theorem. As a start, let me first review some essential aspect of the Bell-theorem that are needed to start this analysis.

The Bell-theorem shows a contradiction between quantum mechanical *statistical* predictions and local realism, i.e. the Bell theorem is proven using a Bell inequality in terms of expectation values which is violated by certain quantum mechanical statistical predictions. Furthermore, no definite predictions (with probability 1) such as in strict (anti-)correlated systems can be used. Only *indefinite predictions* (probabilities) can be used for which the Born rule (postulate 4') is necessary to calculate these quantum mechanical probabilities. Note that the experimental test of the Bell inequality cannot be accomplished in a single run, but is built up with increasing confidence as the number of runs increases. Thus, the following two aspects are found to be essential for the Bell-theorem.

(A) The statistical aspect, i.e. many runs of an experiment are needed to obtain the expectation values in the Bell-inequality.

(B) The probabilistic aspect, i.e. the Born rule (postulate 4') is needed to calculate certain quantum mechanical expectation values.

Aspect (A) deals with experimental implementability, whereas aspect (B) deals with the theoretical derivation of the theorem. It is these two fundamental aspects that are relevant in the Bell-type theorems of Hardy and GHZ. How do these two theorems deal with these two aspects?

In the algebraic theorem of GHZ, both aspects are discarded with. In fact any algebraic theorem discards of both these aspects[11]. The way in which the algebraic Bell-theorems work is as follows. In contradistinction to the original two-particle Bell-theorem, the idea of EPR to turn the exact and definite predictions of quantum mechanics against the claim of its completeness already breaks down

[11] All algebraic theorems against non-contextual hidden variable theories, e.g. local HV-theories, have the same structure. Using a limited amount of quantum structure (i.e postulates 1',2' and 3') a certain hidden variable value assignment is blocked. The first of such an algebraic theorem was published by Bell [16] in his 1966 review paper on Von Neumann's no-go proof using Gleason's theorem for a continuum of projection operators. In doing so Bell anticipated the independent 1967 result of Kochen and Specker[18] who provided the well-known discrete geometrical argument using only a finite number of projection operators that non-contextualist theories of quantum systems in Hilbert spaces of dimensions three and higher are impossible. Harvey Brown [82] has argued for this view very convincingly and consequently he refers to the Kochen Specker result as the Bell-Kochen-Specker theorem (BKS). David Mermin [29] followed Brown in this terminology.

These original algebraic theorems had to do with contextuality. However there is also a relationship between the algebraic method of these theorems and the question of locality. This connection between non-locality and the BKS-theorem, i.e. between local HV-theories and the purely algebraic structure of quantum mechanics, is first investigated in print by Heywood and Redhead [31]. But it was GHZ who proved the first pure algebraic theorem against local HV theories.

in these algebraic Bell-theorems at the stage of defining elements of reality, i.e. at the stage of the value assignment. The contradiction amounts to showing that two unequal numbers, such as zero and one are equal. Consequently the desired hidden variable construction does not even get off the ground because of algebraic inconsistency, hence the name 'algebraic proof'. The Born rule is not used and consequently a test of the predictions in the GHZ theorem does not need statistics to be tested. In principle[12] only single runs of the experiment are needed for the experimental implementation. After an initial few runs of the experiment, depending upon the outcome, an 'all or nothing' situation then arises which can subsequently be decided by a single run.

In the Bell-theorem without inequalities of Hardy, aspect (A) is discarded with but aspect (B) is maintained. In fact any Bell-theorem[13] without inequalities discards with aspect (A) but maintains aspect (B). The way these Bell theorems without inequalities work is as follows. Using the Born rule a set of probabilistic predictions are obtained. These predictions cannot be modeled by a local HV-theory because a contradiction arises between the quantum mechanical predictions and the local realistic predictions. The experimental implementation is as follows. There is no need for statistical data gathering to test some bound on predicted expectation values. Rather, once certain results are observed, the contradiction in the local HV theory can arise with certainty out of some single other observed result. However this other result, only arises with a certain probability. Thus with a certain probability an 'all or nothing' situation arises in which local realism and quantum mechanics contradict each other[12]. For this reason the Bell-theorems without inequalities are also called *quasi-algebraic*.

These preliminary statements about the two theorems will be made more explicit below, but before going any further into the specific theorems, I will define them.

Definition 4.3.1 (Bell-theorem without inequalities). *A Bell-theorem without inequalities is a Bell-theorem that does not use a statistical inequality in terms of expectation values in order to get a violation between local realism and quantum mechanics. (Note that this theorem has the same logical reach as the original Bell-theorem.)*

Definition 4.3.2 (Algebraic Bell-theorem). *An algebraic Bell-theorem is a Bell theorem not using the Born rule (postulate 4'). More explicitly, the doctrine of local realism (definition 4.2.3) cannot meet the (extended) quantum postulates 1', 2', and 3' of orthodox quantum mechanics.*

Now that these definitions are given, let's look at specific examples by GHZ and Hardy of proofs of each of these theorems. The proof of the original Bell theorem has already been given in section 4.2.5, and the proofs of the other two follow below. At the end of this section these three theorems will be compared and judged according to their logical strength and physical relevance.

[12] Although in principle an 'all or nothing' situation can arise, in practise this might not be possible. See the critique about the experimental implementation of at the end of this section.

[13] Hardy's theorem is not the only Bell-theorem without inequalities. See footnote 15 for a short historical overview of these type of inequalities.

4.3.1 Algebraic Proof: GHZ-Theorem

In 1989 Greenberger, Horne and Zeilinger (GHZ) [27] published the first[14] algebraic proof of the Bell-theorem. In comparison to other formulations of the Bell-theorem it has attracted wide attention mainly because of its logical simplicity and presumed good experimental implementability. The original GHZ proof of 1989 gave rise to some reformulations and related proofs - called GHZ-type proofs - of which the one by Mermin [29] will be here discussed.

Let me first present the formal structure of GHZ-type arguments that provide an algebraic proof. Following Fleming [30] I consider three mutually commuting pairs of self-adjoint operators such that within each pair the operators anticommute. Suppose we take the pairs (A_i, B_i), $i = 1, 2, 3$ with the desired property that

$$[A_i, A_k] = [A_i, B_k] = [B_i, B_k] = 0 \quad \text{for} \quad i \neq k \tag{4.30}$$

and

$$\{A_i, B_i\} = 0 \qquad \forall i. \tag{4.31}$$

Now construct new operators C_i and C_0 in the following way

$$C_i = A_i B_j B_k \qquad i \neq j, j \neq k, i \neq k, \quad i = 1, 2, 3 \tag{4.32}$$
$$C_0 = A_1 A_2 A_3 \tag{4.33}$$

The following crucial observations allow for the GHZ-argument to take place. Firstly, the operators C_i (i=1,2,3) and C_0 are all mutually commuting and thus possess simultaneous eigenvectors. Furthermore, each C_i is composed out of mutually commuting operators. The C operators obey the following relation

$$C_1 C_2 C_3 = -C_0, \tag{4.34}$$

and the product of the four C operators satisfies

$$C_0 C_1 C_2 C_3 = A_1 A_2 A_3 A_1 B_2 B_3 A_2 B_3 B_1 A_3 B_1 B_2 = - A_1^2 A_2^2 A_3^2 B_1^2 B_2^2 B_3^2 \leq 0. \tag{4.35}$$

From this last observation it follows that the eigenvalues and the expectation values of $C_0 C_1 C_2 C_3$ must always be non-positive.

The desired contradiction now follows if we assume non-contextual possessed values for the observables represented by all of the A, B and C operators. Write these possessed values as a_i, b_j, c_k, etc. Because the composition of the C operators is in terms of mutually commuting A and B operators, the possessed values for the observables represented by the C operators are given by:

$$c_i = a_i b_j b_k \qquad i \neq j, j \neq k, i \neq k, \quad i = 1, 2, 3 \tag{4.36}$$
$$c_0 = a_1 a_2 a_3 \tag{4.37}$$

[14] In 1966 John Bell[16] and in 1967 Kochen and Specker[18] published the the first algebraic proof against *g*eneral non-contextual HV theories, GHZ provided the first algebraic theorem explicitly for HV models that assumed local realism to *p*hysically motivate the non-contextualism of the HV models.

Because the product of the C operators consists out of mutually commuting self-adjoint operators, it itself is self-adjoint and thus represents an observable. Requiring non-contextual possessed values for this observable implies that these values are given by the product of the possessed values for the C observables. We then find

$$c_0c_1c_2c_3 = a_1a_2a_3a_1b_2b_3a_2b_3b_1a_3b_1b_2 = +a_1^2a_2^2a_3^2a_1^2b_2^2b_3^2 \geq 0 \tag{4.38}$$

and the possessed values of $C_0C_1C_2C_3$ must always be positive. Following the hidden variable program, assume that the possessed values for any observable are restricted to the eigenvalues of the representing operator. But then the above results of Eq.(4.35) and Eq.(4.38) are only consistent iff the product of the C operators is always zero. However, this implies that at least one of the A or B operators is zero. The desired contradiction is now arrived at for any instance of A and B in which none of them has a zero eigenvalue.

In the argument of GHZ [27, 28] and Mermin [29] a physically interesting instance is given that provides such a contradiction. The interesting thing about this argument is that the assumption of non-contextual possessed values for the C operators and their products was eliminated using a locality assumption. They apply the C operators to a simultaneous eigenstate of these operators that has eigenvalues ± 1 and further they let the subscripts of the A and B operators refer to spatially separated particles so that they can use locality (i.e. a local deterministic HV theory) to assign non-contextual possessed values in the way it was done in Eq. (4.38). They use a deterministic HV theory because the measurement results themselves have to be determined by the HV theory instead of only the probability to obtain these results. See also footnote 8.

The physical system both Mermin and GHZ use is a spatially separated three particle system where each particle has spin $\frac{1}{2}$. The operators A_i and B_j are then taken to be the spin-operators σ_x^i and σ_y^j respectively with eigenvalues ± 1. Then the C operators are the following mutually commuting self-adjoint operators (where I have omitted the tensor product sign $\otimes$):

$$\sigma_x^1\sigma_y^2\sigma_y^3 \qquad \sigma_y^1\sigma_x^2\sigma_y^3 \qquad \sigma_y^1\sigma_y^2\sigma_x^3 \qquad \sigma_x^1\sigma_x^2\sigma_x^3. \tag{4.39}$$

Here the subscript $1, 2, 3$ refers to the different three particles. The specific three-particle eigenstate of these three operators is the so-called GHZ-state:

$$|\,\psi\rangle_{GHZ} = (|\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\rangle)/\sqrt{2}. \tag{4.40}$$

where $|\uparrow\rangle$ specifies spin-up and $|\downarrow\rangle$ specifies spin-down along the appropriate z axis. Because this state is an eigenstate of the four spin operators, we get that the product of the measurement results is determined by quantum mechanics. A measurement on two particles thus determines the value of the observable that is measured on the third particle. This means that, according to quantum mechanics, for the measurement of $\sigma_x^1\sigma_y^2\sigma_y^3$, the joint probability to obtain the third outcome given the first two outcomes must give the following result: $p_{xyy}(a, b, c|a, b) = 1$, where the product abc must equal 1.

Now assume local realism and thus factorisability for all joint probabilities of the spatially separated systems. Then we have the following result

$$p_{xyy}(a, b, c|a, b, \lambda) = p_x(a|a, \lambda)p_y(b|b, \lambda)p_y(c|\lambda) = p_y(c|\lambda) = 1, \tag{4.41}$$

with $abc = 1$. Similar results hold for all the other measurements. Here λ is the hidden variable for the specific measurement outcome as determined by the HV-theory. From this result we see that the outcome for the third particle of the measurement of the spin in the y-direction has probability equal to 1 and is thus completely determined. In other words, according to local realism the spin value for this particle in the y-direction has a definite value, say $v(\sigma_y^3)$, that is independent from both the other measurement setups and outcomes of the other two particles, i.e. it can be considered a non-contextual possessed value. Using a similar reasoning it can be shown that if one assumes local realism one can assign to each particle a well-defined possessed spin-value $v(\sigma_x)$ and $v(\sigma_y)$ in respectively the x- and y-direction. Then the value assignments for the tri-partite observables factorise, e.g.

$$v(\sigma_x^1\sigma_y^2\sigma_y^3) = v(\sigma_x^1)v(\sigma_y^2)v(\sigma_y^3), \tag{4.42}$$

and similarly for the other three operators of Eq.(4.39).

Using this local realistic reasoning it is possible to get a value assignment of the spin observables in the GHZ-state such that the above constructed contradiction in terms of the C operators follows. To see this consider the product of the four spin operators of Eq.(4.39). This product is again a self-adjoint operator that commutes with all four spin operators. It has the following property:

$$(\sigma_x^1\sigma_y^2\sigma_y^3)(\sigma_y^1\sigma_x^2\sigma_y^3)(\sigma_y^1\sigma_y^2\sigma_x^3)(\sigma_x^1\sigma_x^2\sigma_x^3) = -[(\sigma_x^1\sigma_x^2\sigma_x^3)(\sigma_y^1\sigma_y^2\sigma_y^3)]^2 \leq 0. \tag{4.43}$$

Thus this product operator must have a negative eigenvalue, and in the GHZ state it is equal to -1. However, if one supposes that each spin component in the x and y direction of the three-particles has a fixed value $v(\sigma_x)$ and $v(\sigma_y)$, as is determined by a local deterministic HV theory, then the product of the possessed values corresponding to the spin observables in Eq.(4.43) for the GHZ state gives the value $+1$. This can be seen as follows [29]. From the assumption that the spin values of each particle all have a fixed value, it follows that for any system in the state $|\psi\rangle_{GHZ}$ the results of whichever of the four sets (xyy, yxy, yyx, xxx) of different three single-particle spin measurements on chooses to measure are specified. Because $|\psi\rangle_{GHZ}$ is an eigenstate of $\sigma_x^1\sigma_y^2\sigma_y^3$, $\sigma_y^1\sigma_x^2\sigma_y^3$, $\sigma_y^1\sigma_y^2\sigma_x^3$, and $\sigma_x^1\sigma_x^2\sigma_x^3$ with eigenvalues 1, 1, 1 and -1, the product of the four trios of 1's and -1's must obey the following relations:

$$\begin{aligned} &v(\sigma_x^1)v(\sigma_y^2)v(\sigma_y^3) = 1, \quad v(\sigma_y^1)v(\sigma_x^2)v(\sigma_y^3) = 1, \\ &v(\sigma_y^1)v(\sigma_y^2)v(\sigma_x^3) = 1, \quad v(\sigma_x^1)v(\sigma_x^2)v(\sigma_x^3) = -1 \end{aligned} \tag{4.44}$$

However, these relations are mutually inconsistent because the product of the four left sides is necessarily $+1$. The same contradiction can be seen when we use the factorisable value assignment determined by the local HV-theory for Eq.4.43:

$$\begin{aligned} &v(\sigma_x^1\sigma_y^2\sigma_y^3\sigma_y^1\sigma_x^2\sigma_y^3\sigma_y^1\sigma_y^2\sigma_x^3\sigma_x^1\sigma_x^2\sigma_x^3) = \\ &v(\sigma_x^1\sigma_y^2\sigma_y^3)v(\sigma_y^1\sigma_x^2\sigma_y^3)v(\sigma_y^1\sigma_y^2\sigma_x^3)v(\sigma_x^1\sigma_x^2\sigma_x^3) = \\ &[v(\sigma_x^1)v(\sigma_y^2)v(\sigma_y^3)][v(\sigma_y^1)v(\sigma_x^2)v(\sigma_y^3)][v(\sigma_y^1)v(\sigma_y^2)v(\sigma_x^3)][v(\sigma_x^1)v(\sigma_x^2)v(\sigma_x^3)] = \\ &[v(\sigma_x^1)v(\sigma_y^1)v(\sigma_x^2)v(\sigma_y^2)v(\sigma_x^3)v(\sigma_y^3)]^2 = 1 \end{aligned} \tag{4.45}$$

This is in clear contradiction to the requirement of Eq.(4.43) that it has to be -1. This completes the GHZ argument that a local deterministic HV theory cannot be used to model the predictions of quantum mechanics. Note that no inequality, statistics or probabilistic reasoning is needed.Contrary to the Bell-theorem of section 4.2.5 no statistical correlations for expectation values are used.

Let's go back and ask ourselves what this GHZ argument has proven? In contradistinction to the original two-particle Bell-theorem, the idea of EPR to turn the exact predictions of quantum mechanics against the claim of its completeness already breaks down in this algebraic Bell-theorem at the stage of defining elements of reality, i.e. at the stage of the value assignment. Thus the premises of local realism when applied –using a certain Quantum-criterium– to a system of three spin-$\frac{1}{2}$ particles are inconsistent. In the Bell-theorem which uses only two spin-$\frac{1}{2}$ particles, these premises are not inconsistent but only lead to different result than quantum mechanics. The only things needed for this GHZ argument are (i) certain quantum mechanical operators that are supposed to correspond to observables and whose results upon measurement are supposed to be given by one the eigenvalues of these operators and (ii) a specific value assignment to the outcomes of the observables that is in accordance with local realism. Actually, this is nothing more than the orthodox quantum postulates 1'-3' supplemented with the assumption of a local deterministic HV theory. In other words, the GHZ-argument constitutes an algebraic Bell-theorem:

Theorem 4.3.1 (GHZ-theorem). *A local deterministic HV-theory cannot meet the orthodox quantum postulates 1' to 3'.*

Note that the quantum postulate 4', the so-called Born-rule, that specifies the probability for a certain result to be found upon measurement is not needed. Further, the GHZ theorem requires a deterministic HV theory because the value assignment it uses for the HV theory determines uniquely the results upon measurement. This deterministic theory is needed because the argument requires the usage of the perfect correlations, i.e. the complete anti-correlations, of the GHZ-state. If less correlated states (non-maximally entangled states) are used then the GHZ argument does not go through. Lastly, whereas Bell needed the extension beyond the strict correlation measurements to show inconsistency of quantum mechanical statistical predictions with local realism, note that this argument requires only the perfect correlation measurements. In the words of GHZ this constitutes 'the most significant feature' of their argument, i.e "that the EPR-program [local realism] cannot handle even the perfect correlations of quantum mechanics for systems of three or more particles. [28]".

4.3.2 A Halfway House: Hardy's Proof without Inequalities

In 1992 Hardy [34] has published an interesting proof that local realism is in conflict with the predictions of quantum mechanics. He proved that *any* system consisting of two spin-1/2 particles in a non maximally entangled state allows for a Bell-theorem not involving inequalities. This proof is halfway in between the original proof by Bell and the proof by GHZ. To be more specific, no inequality like the CHSH inequality is needed, but whereas the GHZ argument does not need probabilistic reasoning (i.e. the Born rule), the Hardy-argument does. It uses the Born rule to calculate quantum mechanical probabilities and is thus not an algebraic proof. Hardy's argument is thus a case of a 'Bell-theorem without inequalities' and although it was not the first to appear in the quantum literature[15] it nevertheless attracted wide attention, partly because of its great presumed experimental implementability.

Let me first present the formal structure of the Hardy-type arguments [35, 38]. Consider two particles emitted in two spatially distinct directions towards measurement apparatuses. On both particles two dichotomous observables are measured that are represented by A_k and B_k where $k = 1$ for the first particle and $k = 2$ for the second particle. The results of the measurements are either 1 or 0. Hardy now has proven that for a specific set of states the following predictions hold in quantum mechanics:

$$\mathrm{A}_1 = 1 \text{ and } \mathrm{A}_2 = 1 \text{ happens sometimes.} \tag{4.46}$$

$$\text{If } \mathrm{A}_1 = 1 \text{ then } \mathrm{B}_2 = 1. \tag{4.47}$$

$$\text{If } \mathrm{A}_2 = 1 \text{ then } \mathrm{B}_1 = 1. \tag{4.48}$$

$$\mathrm{B}_1 = 1 \text{ and } \mathrm{B}_2 = 1 \text{ never happens .} \tag{4.49}$$

At first glance these predictions appear contradictory. For suppose that in an experiment both A_1 and A_2 are measured and found to be 1. This is in accordance with Eq. 4.50. From Eq. 4.47 and the result $A_1 = 1$ follows that $B_2 = 1$ and similarly from Eq. 4.48 and the result $A_2 = 1$ follows that $B_1 = 1$. But this contradicts Eq.(4.53). As we will see, the only resolution for this apparent contradiction is to assume contextuality and because we are dealing with spatially distinct particles this amounts to assuming some form of non-locality. Before going into this question of non-locality, I will first show how the above mentioned predictions follow from quantum mechanics.

An equivalent way of formulating these predictions in terms of quantum mechanical expectation values of projection operators A_k and B_K is as follows:

$$\langle A_1 \otimes A_2 \rangle > 0, \tag{4.50}$$

$$\langle A_1 \otimes (\mathbb{1} - B_2) \rangle = 0, \tag{4.51}$$

$$\langle (\mathbb{1} - A_1) \otimes B_2 \rangle = 0, \tag{4.52}$$

$$\langle B_1 \otimes B_2 \rangle = 0. \tag{4.53}$$

There is a whole set of states that obeys these equations, which Hardy was the first to construct. I will here present this construction.

Each particle is assumed to have a two-dimensional Hilbert space as its state space. Now two sets of orthonormal basis vectors for each of these two Hilbert spaces which are denoted by $\{|\, x_k\rangle \,, |\, y_k\rangle\}$ and $\{|\, u_k\rangle \,, |\, v_k\rangle\}$ with $k = 1, 2$ for

[15] Actually Heywood and Redhead published the first Bell theorem without inequalities in 1983, but this was not taken up by the physics community, partly because of the difficult formulation. This result was greatly simplified in 1983 in an article by Stairs [32], however the article was on quantum logic and it appeared in a philosophical journal instead of a physics journal and remained thus as good as unknown. In 1990 Brown and Svetlichny [33] presented the argument of Stairs in a paper that was explicitly dealing with the Bell-theorems without inequalities and thus opened the way for the rest of the physics community to get to know these sorts of theorems.

respectively particle 1 and 2. The basis vectors are related to each other in the following way:

$$
\begin{aligned}
|\,x_k\rangle &= d\,|\,u_k\rangle + f\,|\,v_k\rangle && (4.54)\\
|\,y_k\rangle &= f^*\,|\,u_k\rangle - d^*\,|\,v_k\rangle && (4.55)
\end{aligned}
$$

where the coefficients are formalised, $|d|^2 + |f|^2 = 1$ and $0 < |d| < 1$, $0 < |f| < 1$. The operators A_k and B_K are taken to correspond to the projection operators:

$$
A_k = |\,y_k\rangle\,\langle\,y_k| \quad \text{and} \quad B_k = |\,u_k\rangle\,\langle\,u_k|\,. \tag{4.56}
$$

Now the set of two particle states we are looking for is:

$$
|\,\psi\rangle = M(|\,x_1\rangle\,|\,x_2\rangle - d^2\,|\,u_1\rangle\,|\,u_2\rangle) \tag{4.57}
$$

with M an normalization constant. Because $0 < d < 1$ this state is never a maximally entangled state, i.e. it cannot be transformed into the single state. This state has the following four equivalent forms:

$$
\begin{aligned}
|\,\psi\rangle &= M(df\,|\,u_1\rangle\,|\,v_2\rangle + df\,|\,v_1\rangle\,|\,u_2\rangle + f^2\,|\,v_1\rangle\,|\,v_2\rangle) && (4.58)\\
|\,\psi\rangle &= M(|\,x_1\rangle\,(d\,|\,u_2\rangle + f\,|\,v_1\rangle) - d^2(d^*\,|\,x_1\rangle + f\,|\,y_1\rangle)\,|\,u_2\rangle) && (4.59)\\
|\,\psi\rangle &= M((d\,|\,u_1\rangle + f\,|\,v_1\rangle)\,|\,x_2\rangle - d^2\,|\,u_1\rangle\,(d^*(|\,x_2\rangle + f\,|\,y_2\rangle)) && (4.60)\\
|\,\psi\rangle &= M(|\,x_1\rangle\,|\,x_2\rangle - d^2(d^*\,|\,x_1\rangle + f\,|\,y_1\rangle)(d^*(|\,x_2\rangle + f\,|\,y_2\rangle)). && (4.61)
\end{aligned}
$$

Using these four state formulations, it can be easily checked that this set of states together with the operators A_k and B_k reproduces Eq.(4.50) - Eq.(4.53) as long as A_k and B_k do not commute and the coefficients d and f are nonzero. Note that in order to check this, one needs to use the quantum postulates 1' to 4' of the orthodox formalism. Using Eq.(4.58) we see that if we measure B_1 and B_2 then $\langle B_1 B_2\rangle = 0$. From Eq.(4.59) it follows that if we measure A_1 and B_2 then if $A_1 = 1$ then $B_2 = 1$. Similarly from Eq.(4.60) it follows that if we measure B_1 and A_2 then if $A_2 = 1$ then $B_1 = 1$. Lastly, from Eq.(4.61) we see that if we measure A_1 and A_2 then for these experiments $A_1 = 1$ and $A_2 = 1$ with probability $|Md^2 f^2|^2 > 0$ which confirms prediction (4.50). The set of states of Eq.(4.57) are called *Hardy-states.*

After having shown that quantum mechanical states exist that can meet Eq.(4.50) - Eq.(4.53), let' s go back to the apparent contradiction that these equations give rise to and show that it is the implicit assumption of local realism that gives rise to this contradiction. Let me employ a hidden variables formalism with hidden variables $\lambda \in \Lambda$. Prediction (4.50) gives: $\mathbb{P}^{\mathrm{lr}}(A_1 = 1\,\&\,A_2 = 1) \neq 0$. Thus there must exist some $\lambda \in \Lambda'$ in Λ for which $\mathbb{P}^{\mathrm{lr}}(A_1 = 1\,\&\,A_2 = 1|\lambda) \neq 0$. The size of the subset Λ' is not important. Now assume local realism, i.e. use factorisability of Eq.(4.93) for all probabilities. This implies:

$$
\mathbb{P}^{\mathrm{lr}}(A_1 = 1|\lambda) \neq 0 \text{ and } \mathbb{P}^{\mathrm{lr}}(A_2 = 1|\lambda) \neq 0 \qquad \text{for } \lambda \in \Lambda'. \tag{4.62}
$$

From prediction (4.47) it now follows that: $\mathbb{P}^{\mathrm{lr}}(A_1 = 1\,\&\,B_2 = 0) = 0$, and thus for all $\lambda \in \Lambda'$: $\mathbb{P}^{\mathrm{lr}}(A_1 = 1\,\&\,B_2 = 0|\lambda) = 0$. Using factorisability again this reduces to: $\mathbb{P}^{\text{lr}}(A_1 = 1|\lambda)\mathbb{P}^{\text{lr}}(B_2 = 0|\lambda) = 0$. Together with (4.62) this gives: $\mathbb{P}^{\text{lr}}(B_2 = 0|\lambda) = 0$ for $\lambda \in \Lambda'$ and consequently:

$$\mathbb{P}^{\text{lr}}(B_2 = 1|\lambda) = 1 \qquad \text{for} \quad \lambda \in \Lambda'. \tag{4.63}$$

Using a similar reasoning it can be shown that

$$\mathbb{P}^{\text{lr}}(B_1 = 1|\lambda) = 1 \qquad \text{for} \quad \lambda \in \Lambda'. \tag{4.64}$$

where we use prediction (4.48). Using these result we see that the results of the B_k measurement are predetermined at the source for a sub-ensemble of cases such that $B_1 = 1$ and $B_2 = 1$. This clearly contradicts prediction (4.53).

Let's go back and ask ourselves what has been proven by this contradiction. It has been shown that the set of predictions of Eq.(4.50) - Eq.(4.53) cannot be modeled by a local realistic theory. In other words, assuming the set of predictions and factorisability –a necessary ingredient of local realism– to model a certain set of predictions leads to a contradiction. However, we have also seen that using the quantum postulates 1' to 4', certain quantum mechanical states and observables could be constructed that do allow for the set of predictions to follow. Thus we have a contradiction between local realism and quantum mechanics, i.e a Bell-theorem.

It is interesting to compare this result to the GHZ-theorem and to the original Bell-theorem that resulted from a violation of the CHSH inequality. The GHZ-theorem can be presented as follows. If local realism holds then in a GHZ type experiment there would be *individual* events that would violate the predictions of quantum mechanics. In the original Bell-theorem it would only be necessary for a *statistical* violation of quantum mechanics. As Hardy himself already noted, the above presented proof falls halfway between these two extremes: "If local realism holds, then either we must have the statistical violation of quantum mechanics that a $A_1 = 1$ and $A_2 = 1$ result is never seen or at least one of the other predictions (4.47)-(4.48) must be violated in a single event (or both) [35]". Once a $A_1 = 1$ and $A_2 = 1$ result is seen the situation becomes an all or nothing situation just like in the GHZ case. Thus, once a certain result is observed the contradiction can arise with certainty out of some other *individual* result. However, this first result only arises with a certain probability. Although no inequality like the CHSH inequality is used, nevertheless probabilistic reasoning was needed using the Born postulate (postulate 4') to run the argument. In conclusion, the above presented Hardy-proof that local realism is in conflict with quantum mechanics is a proof of a Bell-theorem without inequalities, the so-called Hardy-theorem:

Theorem 4.3.2 (Hardy-theorem). *A local HV-theory does not meet the quantum postulates 1' to 4' and no statistical inequalities are needed to test this.*

Now that the final form of the Hardy-theorem has been arrived at, I would like comment on a special feature of the Hardy-theorem that distinguishes it from the Bell-theorem. While in the original formulation of the Bell-theorem by Bell, the maximum discrepancy with local realism occurs for maximally entangled states, the above presented Hardy argument is by contrast not valid for maximally entangled states. Hardy has shown that it only works for *all* non-maximally entangled states [35]. Further, Jordan [38] has proved the converse of this result. He has shown that for any choice of two different measurement possibilities for each particle, a non-maximally entangled state can be found which gives a Hardy-type contradiction. However, Cabello [37] has recently given a Hardy-like argument for a Bell-theorem without inequalities that holds also for maximally entangled states when using four instead of two particles.

4.3.3 Logical and Experimental Strength of the Bell-, Hardy-, and GHZ-theorem

Let me now compare the Hardy-theorem and the GHZ-theorem to the Bell-theorem. The reason behind this is that I would like to comment on Mermin's statement that the Hardy-theorem is the 'best version of Bell's theorem' [39] because according to Mermin it is "by far the simplest and cleanest case" for providing Bell-theorems. Without going into details about what actually constitutes some version to be the *best* version, I would like to distinguish two points of view, a logical and physical point of view, to judge the Hardy-theorem in comparison with the GHZ-theorem and the Bell-theorem.

From a formal *logical point* of view the Hardy-theorem is nothing but the Bell-theorem. Both need the same amount of quantum structure to show an inconsistency of this structure with the same HV-theory. However, the GHZ-theorem requires less quantum structure than the Bell-theorem to show the inconsistency of local realism with quantum mechanics. The Born-rule, postulate 4', is not needed. Because of this the GHZ-theorem is logically stronger than both the Hardy-theorem and the Bell-theorem. Although the Hardy- and Bell-theorem do not use a deterministic HV-theory, but allow for a general stochastic HV-theory, this has no logical implications. Since any non-deterministic theory can be upgraded to a deterministic one (See footnote 8), the GHZ-theorem that does require a deterministic theory is in this respect not weaker.

However, from a *physical*, i.e. *experimental*, point of view the Bell-theorem is superior to both the Hardy-theorem and the GHZ-theorem because it can be more easily experimentally tested whereas the experimental testability of the latter two is problematic. However, at first sight this might appear not to be true. The GHZ theorem states that from three experiments one can predict the outcome of a single other experiment which gives $+1$ for local realism and -1 for quantum mechanics. One then thus gets an 'all or nothing' situation that will be decided by one individual event. The Hardy-theorem also is able to result into such 'an all or nothing' situation that can be decided in one single run of the experiment. When comparing this 'all or nothing' situation to the many runs of experiments needed in the Bell-theorem to get statistics that are significant enough to violate the Bell-inequality, one is tempted to say that both the Hardy-theorem and the GHZ-theorem are experimentally superior to the Bell-theorem. However, I will try to argue that this is not true.

In real experiments, inequalities are necessary to ensure that the errors do not wash out the logical contradiction that local realism faces. However, even if there were no errors, I nevertheless believe that the experimental implementation of both the Hardy theorem and the GHZ theorem cannot be met via individual events but requires many runs of the experiment after which a statistical analysis must be performed. The reason for this is as follows: although the operators considered in the both the GHZ and Hardy argument are mutually commutative, they are however *not* simultaneously measurable and therefore the hidden variables inferred from one group of measurements are incompatible with the results produced by another group of predicted measurements.

From this point of view the GHZ and Hardy refutation are thus actually refutations that use incompatible sets of measurements and such a type of refutation cannot be accomplished in a single run, but is built up with increasing confidence as the number of runs increases. Let me try to explain this claim by looking first at the GHZ argument.

Of course the four observables of Eq.(4.39) used in the GHZ argument are mutually commutative, and no doubt, an operator of the form $\sigma_x^1\sigma_y^2\sigma_y^3$ can be measured by way of a simultaneous separate measurement of the three observables σ_x^1, σ_y^2 and σ_y^3. However, the critique of section 2.8.2 on the standard account of measurement compatibility in quantum mechanics applies equally well here. Again following Harvey Brown, "the root issue is not mathematical commutativity but measurement compatibility, and the former is certainly not a sufficient condition for the latter." [83]. And having this in mind we better ask ourselves: How does one measure the four mutually commuting self-adjoint observables of Eq.(4.39) (that are multiplied to give the large product operator that is mentioned in Eq.(4.43)) using *only* compatible measurements?

I will consider two alternative measurement procedures which are both shown to be fundamentally flawed because of measurement incompatibility. The first procedure is the tempting idea to measure each of the six local observables separately and then take the product of their outcomes in order to get the contradictory results of Eq.(4.44) or of Eq.(4.45). However, this would imply measuring simultaneously mutually non-commutative observables such as σ_x^1 and σ_y^1 which are certainly not compatible. One thus has to use different measurements that each get assigned a unique event number that also characterizes the hidden variable assignment for each value assignment. Thus one would get four different sets of hidden variables $\lambda_i, \lambda_{ii}, \lambda_{iii}$ and λ_{iv} with specific event numbers i to iv for measurements of the four observables of Eq.(4.39). For example, these sets would give rise to the value assignments $v(\sigma_x^1)_i$, and $v(\sigma_x^1)_{ii}$ for measuring the spin-value in the x-direction for the measurement setups of respectively $\sigma_x^1\sigma_y^2\sigma_y^3$ and $\sigma_x^1\sigma_x^2\sigma_x^3$. The contradictory value assignments of Eq.(4.44) and of Eq.(4.45) then can only hold when the event numbers are ignored. However it is improbable that the four sets would coincide and thus this measurement procedure can not give us compatible measurements of the observables needed to run the GHZ argument[16].

Now, as an alternative second procedure let us assume that instead of measuring the six spin-operators individually we will measure the the mutually commuting observables in Eq.(4.39) such as $\sigma_x^1\sigma_y^2\sigma_y^3$ directly so as to make the measurement procedures compatible. Then the value assignment $v(\sigma_x^1\sigma_y^2\sigma_y^3)$ refers to the predicted outcome of some sort of holistic measurement of some non-local observable on system A+B+C, which is (by assumption) compatible with similar measurement operations associated with $v(\sigma_y^1\sigma_x^2\sigma_y^3)$, $v(\sigma_y^1\sigma_y^2\sigma_x^3)$ and $v(\sigma_x^1\sigma_x^2\sigma_x^3)$. In

[16] Belinsky en Klyshko[14] have a similar argument that the GHZ result can have no relation to a real experiment. Using a different argument, they also argue that the only way to run the GHZ argument is to ignore the event numbers for the hidden variable assignment.

the argument it then is assumed that this holistic value $v(\sigma_x^1\sigma_y^2\sigma_y^3)$ coincides with $v(\sigma_x^1)v(\sigma_y^2)v(\sigma_y^3)$ and the argument is carried out. The non-local observables that are now being measured indeed mutually commute, but the root issue is, as stated before, whether or not they are compatible. Can this assumption of compatibility be justified? In other words, can one simultaneously measure these non-local holistic observables?

It is not known how to perform such a holistic measurement and if they are at all possible[17]. But even if they are possible then one may well ask why the value assignment $v(\sigma_x^1\sigma_y^2\sigma_y^3) = v(\sigma_x^1)v(\sigma_y^2)v(\sigma_y^3)$ as used in Eq.(4.45) should hold in this case. I will now argue that, upon the assumption of the existence of non-local (holistic) measurements, there is actually no reason to require that this value assignment must hold for the hidden variable states that one can deduce from the predictions.

In order to run the GHZ argument it is assumed that for value assignments of operators such as for example $A \otimes B \otimes C$ the following holds:

$$v(A \otimes B \otimes C) = v(A)v(B)v(C) \qquad \text{for some } \lambda \in \Lambda, \tag{4.65}$$

for any mutually commuting operators A, B and C, *no matter how* $A \otimes B \otimes C$ is measured. Remember that I assume that the measurement of $A \otimes B \otimes C$ is non-local. One now is reminded [83] of the criticism by Bell of the non-contextualist assumption of Von Neumann (see Eq. (4.7)), that the hypothetical value of an observable should be independent of the manner in which the operator is being measured, in the case where the choice is between mutually incompatible experimental arrangements. In this second measurement procedure the observable is given by the operator $\sigma_x^1\sigma_y^2\sigma_y^3$ (amongst others) and the choice is between the incompatible measurement setups of the non-local measurement of operator $\sigma_x^1\sigma_y^2\sigma_y^3$ and of the separate but simultaneous measurements of σ_x^1, σ_y^2 and σ_x^3.

Having Bell's critique in mind, we see that because of the incompatibility of the measurement procedures one has to use a contextual value assignment such as $v(\sigma_x^1\sigma_y^2\sigma_y^3)_I$ and $v(\sigma_x^1\sigma_y^2\sigma_y^3)_{II}$ where the event number I stands for the holistic measurement procedure of $\sigma_x^1\sigma_y^2\sigma_y^3$ and event number II for the local and separate measurements of σ_x^1, σ_y^2 and σ_y^3 . Since we assume non-local measurements for the joint operators we have to use the value assignment $v(\sigma_x^1\sigma_y^2\sigma_y^3)_I = v(\sigma_x^1\sigma_y^2\sigma_y^3)_{II} = v(\sigma_x^1)_{II}v(\sigma_y^2)_{II}v(\sigma_y^3)_{II}$ which need not hold because of incompatible event numbers. Thus the general value assignment of Eq.(4.65) need not be required to hold for this measurement procedure. This implies that the contradictory results of Eq.(4.45) and of Eq.(4.44) can only be obtained when ignoring these contextual event numbers[18]. To conclude, this second measurement procedure is flawed, because either the holistic measurements needed can not be performed or if they can be performed the required value assignment to run the GHZ argument breaks down because of neglect of measurement compatibility. In this latter case it is impossible, from an experimental point of view, to predict from one measurement

[17] And even if these holistic measurements are possible I believe them to be far more difficult than the relatively simple local measurements in the EPRB-setup to test the Bell-theorem.

[18] Wódkiewicz [84] has shown that it is indeed possible for a local realistic model to give the result of Eq.(4.34) and of Eq.(4.35) when the value assignment $v(\sigma_x^1\sigma_y^2\sigma_y^3) = v(\sigma_x^1)v(\sigma_y^2)v(\sigma_y^3)$ is refuted. He constructed an explicit local realistic model that exactly gives the operator identities of Eq.(4.34) and of Eq.(4.35) when each of the operators of Eq.(4.39) are given their local realistic counterparts.

outcome in a certain setup the results of additional runs of measurements on the system in a different setup to have a certain value. Hence no 'all or nothing' situation as is claimed by GHZ can appear.

Both alternative measurement procedures I just described are seen to be improbable and therefore in my opinion the GHZ argument has no experimental strength. What is needed to save the argument is a formulation in terms of measurable quantities such as expectation values where one does not identify value assignments for incompatible measurement setups. One such formulation is the one Bell used for deriving his own Bell-inequalities.

When we now go to the Hardy theorem we see that same reasoning applies as in the GHZ case. This is because in order to require that the set of predictions of Eq. (4.47)-(4.48) must hold for certain hidden variable states, one has to consider either (i) simultaneous measurement of the non-commutative and thus incompatible A_i and B_i operators –which is clearly not possible– or (ii) one has to consider incompatible measurement setups of holistic and local measurements of amongst others the observable $A_1 \otimes B_2$. Here we see again that measurement incompatibility blocks the experimental implementation of argument. Furthermore, suppose we want to test the Hardy theorem, then the predictions of Eq.(4.50) - Eq.(4.53) have to be checked. But how do you test whether or not something never happens, as is stated in Eq.(4.53)? Presumably by showing that certain coincidence rates are zero. However, this statement invites some thinking about the problematic status of inductive verification. Here I take the stand that this statement is unable to get out of the induction problem and therefore it is impossible to experimentally verify the prediction.

4.4 Extension to N-partite Systems

In this chapter we have so far only seen bi-partite and tri-partite systems. But what about N-partite systems? What do the Bell-type inequalities look like for local HV-theories in the multi-partite case? The extension of the bi-partite case to the multi-partite case will be treated in this section.

This extension is not at all trivial because of the greater complexity of the state space and subsystem structure. The main non-trivial issue is the distinction between full and partial factorisability. Full factorisability is the hypothesis that all marginal probabilities of a large joint probability factorise, i.e. all particles behave locally with respect to each other. And partial factorisability is the assumption that the particles behave locally with respect to some, but not to all other particles. Then, in analogy to the local HV theories tested by the traditional Bell-inequalities that assume full factorisability, one can consider HV theories of N-particle systems in which full and/or partial factorisability is required to hold. An interesting question will then be whether one can show the existence of inequalities that characterize the predictions of all these fully and partially factorisable HV theories. As we will see this question is answered in the affirmative.

In this section, first the extension of bi-partite to N-partite systems for full separability is treated and the question of necessary and sufficient, i.e. complete, sets of Bell-type inequalities for local realism is also addressed. Thus this first subsection deals with the following questions: What is the maximal set of independent inequalities and further what is the set that is both necessary and sufficient for a local HV-model to exist for the correlation tables it wants to model? In the following subsection the extension of full factorisability to partial factorisability in HV-models is performed. Here the so-called Svetlichny inequalities and the partial local hidden variable theories (PLHV) are treated. Lastly, as an application, this new PLHV formalism and its general Svetlichny inequalities is confronted with the structure of the quantum state space. The Svetlichny inequalities are here shown to be sufficient conditions for full N-partite entanglement.

4.4.1 Complete Sets of N-partite Bell-type Inequalities

Measurement Configurations

The CHSH inequality is derived for the most simple case, namely for a bi-partite system with dichotomous observables. I now want to consider more complex situations. Consider an N-partite systems where each of the parties uses m different d-valued observables to perform measurements. See figure 4.3.

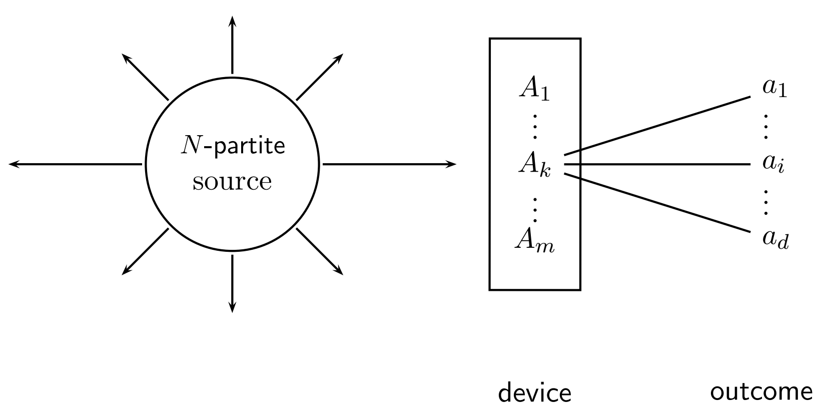


Figure 4.3: General N-partite setup for m d-valued observables.

An interesting way to look at this situation is given by Werner *et al.* [58]: any of the Nm observables divides the hidden variable space Λ into d pieces. The space Λ can now be seen as to be build up out of d^{Nm} regions Λ_γ. Each region is characterized by a single so-called *measurement configuration* γ which is an assignment of one of the d outcomes to each of the Nm observables. As an example (also given by Werner *et al.*.) consider the CHSH case for which we have (N,m,d)=(2,2,2) and a total of $2^{2^2} = 16$ different measurement configurations. Using this notion of measurement configurations to split Λ up into subspaces Λ_γ, Eq.(4.19) expressing factorisability can be re-written as a sum over these subspaces [58]:

$$\mathbb{P}^{\rm lr}(a,b|A,B) = \sum_\gamma \int_{\Lambda_\gamma} d\lambda\, p_A(a|\lambda)p_B(b|\lambda)M(\lambda) = \sum_\gamma p_A(a,\gamma)p_B(b,\gamma)p_\gamma. \quad (4.66)$$

Here $p_\gamma = \int_{\Lambda_\gamma} M(\lambda)d\lambda$ is the probability to obtain the measurement configuration γ. Any expectation values $E^{\rm lr}$ for factorisability are then computed as follows:

$$E^{\rm lr}(A,B) = \sum_{a,b} ab\mathbb{P}^{\rm lr}(a,b|A,B) \quad (4.67)$$

For the general case of N-partite systems the factorisability condition of Eq. (4.66) for joint probabilities becomes the condition of *full factorisability* where each of the subsystems factorises from all the other subsystems:

$$\mathbb{P}^{\rm lr}(a_1,\dots,a_N|A_1,\dots,A_N) = \int_\Lambda d\lambda \prod_i \, p_{A_i}(a_i|\lambda)M(\lambda)$$
$$= \sum_\gamma \int_{\Lambda_\gamma} d\lambda \prod_i \, p_{A_i}(a_i|\lambda)M(\lambda) = \sum_\gamma \prod_i p_{A_i}(a_i,\gamma)p_\gamma \quad (4.68)$$

where a_i is the outcome for measurement of observable A_i.

The measurement configurations γ are an important tool in the construction of Bell-type inequalities as the extreme points of the classically accessible region of the large probability space composed out of all possible response probabilities such as $p_A(a,\lambda)$. This will be the topic of the next section.

Introduction to Complete Sets of N-partite Inequalities

So far we have seen only one constraint on correlations arising from local realism. This is the CHSH inequality of Eq.(4.23). On its own it is a necessary but not sufficient condition for a local HV-model to exist for the specific experimental setup of figure 4.2. This inequality is one specific example of a Bell-type inequality. In general there exists an infinite hierarchy of Bell-type inequalities that can be classified according to the specific type of correlation experiment (i.e. measurement configuration they deal with.

In the next subsections I will discuss the result that for each of the measurement configurations a set of Bell-type inequalities exists that determines the local realistic accessible region of the space of possible outcomes. This set of Bell-type inequalities can be derived from a convexity analysis of the total space of HV-predictions. Peres [78] has shown that obeying these inequalities it is not only a necessary but also a sufficient condition for the existence of a local realistic HV theory.

The hierarchy of inequalities thus obtained all presuppose the existence of local realism for full factorisability. An interesting task is now to find a minimal set of inequalities out of the whole hierarchy which is *complete* in the sense that they are satisfied if and only if the correlations considered allow a local realistic model. The convexity analysis that gives this specific hierarchy of Bell-type inequalities is as follows [58, 78].

Specify the type of correlation measurements one wants to deal with, e.g. consider a N-partite system, where each party can measure m d-valued observables. Then the space spanned by the entire set of raw experimental data is considered, i.e. the space consisting of the $(md)^N$ probabilities. These numbers form a vector ζ in a space of dimension $(md)^N$. This vector is generated by specifying probabilities for each experimental configuration, i.e. for every assignment of one of the values d to each of the mN observables. Note that every configuration γ presents a possible (ideally prepared) state and hence a vector ϱ_γ of probabilities $\mathrm{P}_{\varrho_\gamma}$. The so-called classically accessible region spanned by the vectors ζ is the convex hull of d^{mN} extreme points. This region is thus contained in a convex polytope [58], and is denoted as Ω.

The convex set Ω is the intersection of all half spaces that contain it. Any half space is completely characterised by a linear inequality. Thus we must look for vectors β such that $\langle\beta,\zeta\rangle \leq 1$ for all $\zeta \in \Omega$. This requirement can be checked on the extreme points ϱ_γ and thus we can look at the convex set

$$\mathfrak{C} = \{\beta \mid \forall\gamma : \langle\beta,\varrho_\gamma\rangle \ \leq 1\}. \tag{4.69}$$

This set is also known as the *polar* of $\{\varrho_\gamma\}$. Note the duality between $\mathfrak{C}$ and Ω.

For each $\beta \in \mathfrak{C}$ the inequality $\langle\beta,\zeta\rangle \ \leq 1$ is a necessary condition for $\zeta \in \Omega$. From the Bipolar Theorem it follows that this is also sufficient [58]. Since $\mathfrak{C}$ is convex it suffices to find only its extreme elements. Thus, the classical region is bounded by a finite but very large number of linear inequalities that can be written as $\sum \beta_\gamma \mathrm{P}_{\varrho_\gamma} < M$. These inequalities are the generalizations of the original Bell- and CHSH-inequalities in order to deal with all possible measurement configurations

The problem in construction the hierarchy of inequalities is finding the coefficients β_γ explicitly. This task is closely related to some problems in computational complexity [26] which are very hard to solve.[19] Peres [78] was the first to investigate this. He showed that for any complete set of Bell-type inequalities all the coefficients β_γ can be written in terms of the so-called Farkas vectors. However, the construction of these vectors is rather difficult and no exact solutions were found. Complete solutions only exist either in cases where additional symmetries can be exploited, or for small values of (N, m, d) where computer power can be used for numerical simulation. For example, Pitowsky and Svozil [4] have performed an extensive numerical search for the cases $(N, m, d) = (3, 2, 2)$ and $(2, 3, 2)$. They have obtained the typical result of a list of the coefficients of thousands of inequalities (e.g. 53856 inequalities for the $(3, 2, 2)$ case) from which it is hard to get any insight whatsoever.

Apart from these numerical results, it has been proved only in a few cases that a complete set of Bell-type inequalities exist. In the following subsections these cases will be summarized. The CHSH case will be discussed as the first complete set of inequalities for the case $(N, m, d) = (2, 2, 2)$. Then the extension is made generating N-partite bell-type inequalities. Finally the complete set of inequalities is given for the N-partite case $(N, 2, 2)$. Because of additional symmetries a rather exhaustive discussion is possible for this case.

[19] The general Bell-type inequalities are closely connected to the field of convex geometry. Finding Bell-type inequalities is a special instance of a standard problem in convex geometry known as the *convex hull problem*. This will here not be further investigated, but see Ref.[26] for a thorough investigation.

The Bi-partite CHSH-case

The CHSH inequalities of Eq.(4.23) apply to the measurement configuration $(N, m, d) = (2, 2, 2)$, i.e. two parties with two given dichotomous observables each. Fine [3] was the first to show that these inequalities are complete for this measurement configuration. In particular, he has shown that for this setup the following conditions on correlation tables are equivalent [58]:

1. A local HV-model holds for the correlation table.
2. The CHSH inequalities of Eq.(4.23) hold for all permutations of the observables and outcomes. Thus in total sixteen different CHSH inequalities hold.
3. A joint probability distribution exists for the outcomes of the sixteen observables that returns the correlation probabilities as marginals, i.e. Eq.(4.11) holds for all these observables.

The proof of this equivalence is as follows. In the previous sections conditions 1 and 3 have been shown to be equivalent and implying condition 2. It then remains to show that condition 2 implies the others. This is done by analyzing the classical region bounded by the constraints of local realism, i.e. analyzing the relevant convex polytope [26]. See section 4.4.1 for this type of analysis.

N-partite Bell-type Inequalities for Two Dichotomous Observables per Site

In this section I will discuss one of the first and well-known N-partite Bell-type inequalities. This will be a first step towards the work on complete sets of N-partite Bell-type inequalities. I partly use the formalism of Ref. [58] which uses a terminology and formalism for deriving Bell-type inequalities that will be very useful for later chapters.

Consider an arbitrary N-partite system with two dichotomous observables per site. The relevant data to be considered are the 2^N *full correlation functions* for the 2^N different experimental setups. Each of the setups gets a label determined by the choice of observables at each site. These labels are chosen to be binary variables s_k with $s_k = \pm 1$. The variable s_k indicates the choice of the ± 1-valued observable $A_k(s_k)$ at site k. The full correlation functions are then defined as a specific expectation value of a product of the N observables in the specific experimental setup [20]:

$$\vartheta(s) = E^{\text{lr}}\left(\prod_k A_k(s_k)\right), \tag{4.70}$$

where $s = (s_1, \ldots, s_n)$ is the label for the specific experimental configuration. Note that there are 2^N different configurations.

[20] A 'restricted' correlation function does not use the product of all N signs but the product of subsets of signs, i.e. it considers measurement outcomes of less than N sites.

A very useful way of looking at these full correlation functions $\vartheta(s)$ is to consider them as a component of a vector ϑ in the 2^N-dimensional space spanned by the total experimental data. The Bell-type inequalities are then of the form

$$\sum_s \beta(s)\vartheta(s) \leq 1. \tag{4.71}$$

The coefficients $\beta(s)$ are normalised such that the maximal value for the local realist predictions is 1. For example, for the CHSH inequality we have $\beta(s) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$. The Bell-type inequality of Eq.(4.71) can also be expressed as a bound on the expectation value of

$$\mathfrak{B} = \sum_s \beta(s) \prod_k A_k(s_k). \tag{4.72}$$

Werner et.al. [26] call these expressions *Bell polynomials*. These expressions allow for usage in the quantum case as the so-called *Bell operators*. All observables $A_k(s_k)$ are then substituted by self-adjoint operators $\hat{A}_k(s_k)$ acting on the Hilbert space of the k-th site and the product is the tensor product.

The first solutions found for $\beta(s)$ that gave a bound on some explicit set of Bell-polynomials for $(N, m, d) = (N, 2, 2)$ was found by Mermin [29]. He thereby provided the first Bell-type inequalities in the N-partite case. This inequality was further generalized by Klyshko and Belinsky [10, 98] and Gisin and Bechmann-Pasquinucci [97] through a recursive definition. I will here present this recursive method. Let A_j and A'_j denote dichotomous observables on the j-th particle, $(j = 1, 2, \dots, N)$, and define

$$F_N := \frac{1}{2}(A_N + A'_N)F_{N-1} + \frac{1}{2}(A_N - A'_N)F'_{N-1} \leq 2, \tag{4.73}$$

where F'_{N-1} is the same expression as F_{N-1} but with all A_j and A'_j interchanged. Here, the upper bound on F_N follows by natural induction from the bound on F_2, which is the bi-partite Bell-inequality and thus is equal to 2. One now obtains the so-called Bell-Klyshko inequality [97],

$$|E^{\text{lr}}(F_N)| \leq 2, \tag{4.74}$$

with E^{lr} computed using the factorisable expression of Eq.(4.68). This inequality is a necessary condition any N-partite local HV theory with to exist.

This Bell-Klyshko inequality is also violated in quantum mechanics[21]. That is to say, the expectation value of the corresponding operator

$$\widehat{F}_N := \frac{1}{2}(\widehat{A}_N + \widehat{A}'_N) \otimes \widehat{F}_{N-1} + \frac{1}{2}(\widehat{A}_N - \widehat{A}'_N) \otimes \widehat{F'}_{N-1} \leq 2 \tag{4.75}$$

may violate the bound (4.91) for entangled quantum states. As shown in reference [97], the maximal value is

$$|E_\rho(\widehat{F}_N)| \leq 2^{(N+1)/2}, \tag{4.76}$$

[21] This formulation –of the violation in quantum mechanics of the Bell-Klyshko inequality– has been performed in collaboration with Jos Uffink.

i.e. a violation by a factor $2^{(N-1)/2}$.

The inequality (4.91) can now be extended into a test of $N-1$-entanglement. Consider a state in which one particle (say the N-th) is independent from the others, i.e.: $\rho = \rho_{\{N\}} \otimes \rho_{\{1,\ldots,N-1\}}$. One then obtains:

$$\begin{aligned} |E_\rho(\widehat{F}_N)| &= \left| \mathrm{Tr}\ \rho \left(\frac{1}{2}(\widehat{A}_N + \widehat{A'}_N) \otimes \widehat{F}_{N-1} + \frac{1}{2}(\widehat{A}_N - \widehat{A}'_N) \otimes \widehat{F'}_{N-1} \right) \right| \\ &= \frac{1}{2} \left| \left(\langle \widehat{A}_N \rangle_\rho + \langle \widehat{A}'_N \rangle_\rho \right) \mathrm{Tr}\ \rho \widehat{F}_{N-1} + \left(\langle \widehat{A}_N \rangle_\rho - \langle \widehat{A}'_N \rangle_\rho \right) \mathrm{Tr}\ \rho \widehat{F'}_{N-1} \right| \\ &= \frac{1}{2} \left| \langle \widehat{A}_N \rangle_\rho \left(E_\rho(\widehat{F}_{N-1}) + E_\rho(\widehat{F'}_{N-1}) \right) + \langle \widehat{A}'_N \rangle_\rho \left(E_\rho(\widehat{F}_{N-1}) - E_\rho(\widehat{F'}_{N-1}) \right) \right| \\ &\leq \frac{1}{2} |E_\rho(\widehat{F}_{N-1}) + E_\rho(\widehat{F'}_{N-1})| + \frac{1}{2} |E_\rho(\widehat{F}_{N-1}) - E_\rho(\widehat{F'}_{N-1})| \\ &= \max(|E_\rho(\widehat{F}_{N-1})|, |E_\rho(\widehat{F'}_{N-1})|) \leq 2^{N/2} \end{aligned} \tag{4.77}$$

where it is used that $|\langle \widehat{A}_N \rangle| \leq 1, |\langle \widehat{A'}_N \rangle| \leq 1$ and the bound (4.76).

Since $\widehat{F}_N$ is invariant under a permutation of the N particles, this bound holds also for a state in which another particle than the N-th factorises, and, since $E_\rho(F_N)$ is convex as a function of ρ, it holds also for mixtures of such states. Hence, for every $(N-1)$-particle entangled state we have

$$|E_\rho(\widehat{F}_N)| \leq 2^{N/2}. \tag{4.78}$$

Thus, a sufficient condition for N-particle entanglement is a violation of (4.78), i.e. inequality (4.74) should be violated by a factor larger than $2^{(N/2-1)}$.

N-partite Complete Sets of Bell-type inequalities

Using the formalism of the last subsection Werner and Wolf [26] construct complete sets of Bell-type inequalities for the case $(N, m, d) = (N, 2, 2)$ for full factorisability. These will now be discussed. Although Werner and Wolf were not the first to present single N-partite inequalities, they were, together with Bruckner *et al.* [77], the first to give complete sets. They find the complete sets of solutions for $\beta(s)$ that give the necessary and sufficient set of Bell-type inequalities for local realism to hold.

Any local realistic model must assign probabilities to any collection of values for observables, i.e., to each measurement configuration $s = (s_1, \ldots, s_n)$. Because the extremal assignment of probabilities just assigns probability 1 to one configuration and zero to all others, the extreme elements of the local realistic accessible region Ω are labeled by the experimental configurations s. The task now is to find the extremal linear inequalities $\beta(s)$ of the dual convex space $\mathfrak{C}$ that characterise these extreme points.

In order to get further results it is important to take symmetry considerations into account. The crucial symmetry is the following. Because of the restriction to full correlation functions one can use the invariance of the vector ϑ of Eq.(4.70) under permutation of the values of both observables on two sites. This symmetry leads to the the following result obtained by Werner et.al. Any of the 2^{2^N} binary vectors $f \in \{-1,1\}^{2^N}$ with components $f(r), r \in \{0,1\}^n$ corresponds to one Bell-type inequality via the following expression for $\beta(s)$ of Eq.(4.71):

$$\beta(s) = \frac{1}{2^N} \sum_r f(r)(-1)^{<r,s>}. \tag{4.79}$$

Here $< r, s >= \sum_{i=1}^N r_i s_i$ denotes the inner product.

As proven in [26], these are the coefficients of the complete set of 2^{2^N} extremal Bell-type inequalities specifying the range of expectations of full correlation functions for any local HV-model. Eq.(4.79) gives a complete set of inequalities, in the sense that the considered correlation table allows a local HV-model for full factorisability if and only if all these inequalities are satisfied. It is possible to use a single *non-linear* inequality which is equivalent to the set of 2^{2^N} linear inequalities [26]. However, this gives no further insight and will here thus not be presented.

Note that the symmetry leading to this result is not generic but only valid for the case $(N, m, d) = (N, 2, 2)$. Because of the lack of sufficient symmetry, in general other cases are not easy or perhaps even impossible to solve.

This derivation by Werner, et.al. of the full set of Bell-type inequalities for a local realism is rather abstract and general. A more concrete derivation of the same set of inequalities is given by Bruckner *et al.* [77]. They furthermore show the completeness of the set of inequalities in an explicit constructive way. Nevertheless, the abstract formulation from Werner *et al.* has been presented here, because it sets the formalism and terminology for future results.

4.4.2 Partial Factorisability and Partial Local Hidden Variable Theories

Introduction and concepts.

So far I have only discussed full factorisability for N-partite systems in the local HV-theories. However, the extension from two to N particles also calls for another type of factorisability, the so-called *partial factorisability.*

Definition 4.4.1. Partial factorisability. *Partial factorisability pertains to a system in which subsets of the N parts form extended systems, whose internal states can be correlated in any way (e.g. entangled), which however behave factorisable (e.g. local) with respect to each other*[22]. *For a mathematical formulation of this definition see Eq. (4.86).*

The discrimination of different types of factorisability calls for a further discrimination of the different types of HV-theories for which each of the types of factorisability are assumed to hold. We have already seen the HV-theories for full factorisability, but the ones for partial factorisability –the so-called *partial local hidden variable theories*– are still to be investigated. Let me first define them.

[22] Partial factorisability is also called partial separability. Indeed, in the few papers that have appeared on this subject [23, 93, 92, 11] one always speaks of partial separability. However, for consistency in the terminology, I will not call it this way but refer to partial factorisability. Separability is a concept here defined only in terms of the structure of quantum states and not in terms of the structure of the hidden variable formalism.

Definition 4.4.2. Partial local hidden variable theory (PLHV-theory). *A HV-theory in which partial factorisability holds (and not full factorisability)*[23].

In these theories 'partial' refers to the allowance of the assignment of local hidden variables to certain subsets of the particles and not necessarily to each particle alone. These partial hidden variables only determine the behavior of the extended entities that behave locally in relation to each other. So for example, in the case of a tri-partite state, two locally related subsets can be distinguished of two and one particles respectively, where the subset consisting of two particles could be non-locally related, e.g. possibly entangled.

The idea of partial factorisability is visualized in figure 4.4. In this figure we see three cases, namely for $N = 2$, 3 and 11. For the bi-partite case, figure 4.4a, one has only two options, *either* the two party system is fully factorisable *or* it is non-factorisable. However this only holds for the bi-partite systems. In multi-partite systems one has to consider partial factorisability. For example, as we can see in figure 4.4b in the tri-partite case this results in an extra option in which the system is divided up into two-subsystems of one and two particles respectively that are factorisably related, whereas the bi-partite subsystem does not necessarily have to factorise. For a greater number of particles one has many more possibilities. In figure 4.4c, one of them is drawn for the case of $N = 11$ and some partition of the eleven particles into four subsystems.

In analogy to the standard local HV-theory for whose existence the full set of Bell-type inequalities of Eq. (4.79) are a sufficient and necessary condition, one can ask for sufficient and possibly even necessary conditions for a partial local hidden variable theory to exist. In other words, do inequalities exist that characterize the predictions of all PLHV-theories for the systems under consideration? And if so, what do they look like?

In 1987 George Svetlichny was the first to consider these questions for the case of three particles. He derived two inequalities to distinguish between tri-partite states that are completely non-factorisable and states that allow for a certain decomposition into (partially) factorisable mixtures. The inequalities he derived can detect tri-partite systems that cannot be reduced to mixtures of locally related subsystems. Using the inequalities which Svetlichny derived, one is able to test all non-trivial hidden-variable theories that allow for this three-particle partial factorisability but not for the full factorisability.

Subsequently, very recently these inequalities were generalized by both the author and Svetlichny[93] and by Mitchell *et al.*[13] to $N-$partite systems, i.e. inequalities were derived that characterize the predictions of all partially separable HV theories. The original tri-partite inequality and the recent N-partite inequalities will now be presented.

[23] An example of partial local hidden variable theory is the idea of *macroscopic local realism* as used by Reid [21]. This allows for micro- or meso-states to be non-locally related but macroscopically factorisability is required, i.e. only elements of reality are implied that have macroscopic values. Thus a partial local hidden variable theory and macroscopic local realism allow for subsystem non-locality but do not allow for full (macroscopic) non-locality of the total system.

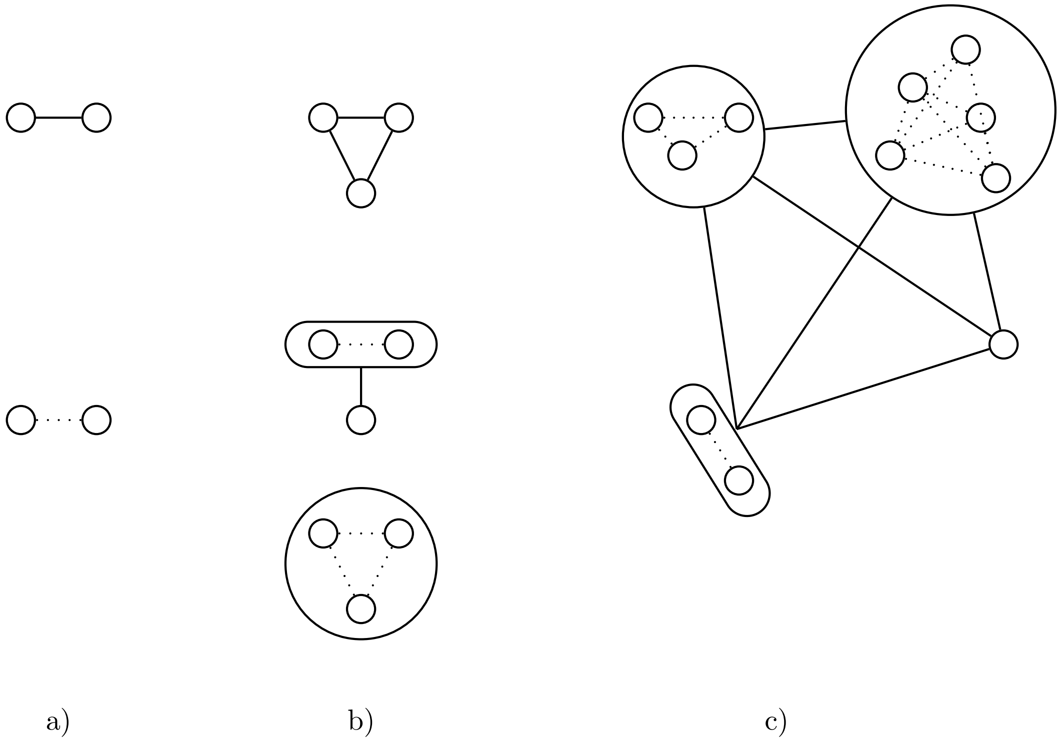


Figure 4.4: Types of correlations. The straight lines represents local (factorisable) correlations and the dotted lines represent correlations that can in principle be anything, e.g. non-local, entangled or local. Here we see three cases: a) bi-partite possibilities, b) tri-partite possibilities, c) example of an N-partite configuration for $N = 11$.

Svetlichny inequalities for tri-partite dichotomous systems.[24]

Svetlichny [23] published inequalities which can detect three-particle correlations that cannot be reduced to mixtures of locally (factorisably) related many-particle subsystems with a fewer number of particles. These inequalities are necessary conditions for all tri-partite PLHV-theories. As will be shown this partial factorisability analysis also provides experimentally accessible sufficient conditions for full tri-partite entanglement, i.e. it distinguishes between three-particle states that are three-particle entangled and those that can be reduced to a mixture of two-particle entangled states (or non-entangled states)[25].

Svetlichny considered a hidden variable model with partial factorisability (PLHV-model), in which for example the third particle behaves independently of the subsystem formed by the other two, see figure 4.4b. This means that, if A, B and C denote dichotomous observables on each of the three particles separately, the following partial factorisable assumption is made for the probability $p_{ABC}(a, b, c)$

[24]This subsection is taken from the first draft of the article by Seevinck and Uffink [92].

[25] Not only was Svetlichny the first to derive inequalities to distinguish between three-and two-particle entanglement, he already used the GHZ state $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\rangle)$ (up to a change of basis) to show that quantum mechanics admits three-particle entangled states.

of the outcomes a, b and c of these observables:

$$p_{ABC}(a,b,c) = \int_\Lambda p_{AB}(a,b|\lambda)p_C(c|\lambda)\mu(\lambda)d\lambda. \tag{4.80}$$

The expected value $E(ABC)$ of the product of the three observables then takes the form $E(ABC) = \int u(A,B|\lambda)v(C|\lambda)d\rho(\lambda)$ where $|u(A,B|\lambda)| \leq 1$ and $|v(C|\lambda)| \leq 1$. Assuming that this form holds for the expectation values $E(A_iB_jC_k)$ for a range of dichotomous observables $A_1, A_2, \ldots; B_1, B_2, \ldots; C_1, C_2, \ldots$, one can derive inequalities of the form $\sum_{ijk} C_{ijk}E(A_iB_jC_k) \leq M$. Svetlichny obtains the following two inequalities, which I call the *Svetlichny inequalities*, for the simplest case of choosing $A_i \in \{A, A'\}$, $B_j \in \{B, B'\}$ and $C_k \in \{C, C'\}$:

$$\begin{aligned} &|\, E(ABC) + E(ABC') + E(AB'C) + E(A'BC) \\ &\quad -E(AB'C') - E(A'BC') - E(A'B'C) - E(A'B'C')\,| \;\leq\; 4, \end{aligned} \tag{4.81}$$

$$\begin{aligned} &|\, E(ABC) - E(ABC') - E(AB'C) - E(A'BC) \\ &\quad -E(AB'C') - E(A'BC') - E(A'B'C) + E(A'B'C')\,| \;\leq\; 4. \end{aligned} \tag{4.82}$$

These inequalities are necessary conditions for all tri-partite PLHV-theories.

The inequalities hold also for three-particle *quantum states* which are two-particle entangled (and non-entangled). Indeed, if we choose Λ as the set of all states on Hilbert space $\mathcal{H}$ of the system and $\mu(\lambda) = \delta(\lambda - \lambda_0)$ where λ_0 is a state of the form

$$\lambda_0 = \rho^{(12)} \otimes \rho^{(3)}, \tag{4.83}$$

we recover the factorisability condition of Eq. (4.80):

$$p_{ABC}(a,b,c|\lambda_0) = p_{\rho^{(12)}}(a,b)p_{\rho^{(3)}}(c), \tag{4.84}$$

where $p_{\rho^{(12)}}$ and $p_{\rho^{(3)}}$ the corresponding (joint) quantum mechanical probabilities to obtain a, b and c for measurements of observables A, B and C. The expectation value $E(ABC)$ then becomes the quantum mechanical expression: $E_{\lambda_0}(ABC) = \mathrm{Tr}[\lambda_0\, A \otimes B \otimes C] = \mathrm{Tr}[\rho^{(12)}\, A \otimes B]\mathrm{Tr}[\rho^{(3)}\, C]$. Thus the same bound as in Eq. (4.81),(4.82) holds also for the quantum mechanical expectation values for a state of the form (4.83). Again, by permutation symmetry and convexity, the same bound holds also for mixed states of the form

$$\rho = p_1\, \rho^{(12)} \otimes \rho^{(3)} + p_2\, \rho^{(13)} \otimes \rho^{(2)} + p_3\, \rho^{(1)} \otimes \rho^{(23)}. \tag{4.85}$$

In other words, it holds for all states which are not three-particle entangled. Violation of inequalities (4.81) and/or (4.82) is thus a sufficient condition for three-particle entanglement[26]. Recently, Svetlichny and I have also obtained similar inequalities for N=4 and higher[93]. These will be presented in the next subsection.

[26] In Ref. [12] of Mitchell *et al.* this same result is obtained.

Generalized Svetlichny Inequalities

In this section the results of the article by Svetlichny and the author [93] is summarized[27]. We obtain necessary conditions for *any* PLHV theory to hold, i.e. inequalities are presented that in an N-particle system can detect N-particle correlations that cannot be reduced to mixtures of locally related many-particle subsystems with a fewer number of particles. I call them here the Svetlichny inequalities. This result is a generalization of the previous section from 3-particle to N-particle systems. In the next subsection this generalization is supplemented with an application of the results to N-partite (entangled) quantum systems.

Imagine a system decaying into N particles which then separate in N different directions. At some later time we perform dichotomous measurements on each of the N particles, represented by observables $A^{(1)}, A^{(2)}, \ldots A^{(N)}$, respectively, with possible results ± 1. Let us now make the following hypothesis of *partial separability*: An ensemble of such decaying systems consists of subensembles in which each one of the subsets of the N particles form (possibly entangled) extended systems which however behave locally with respect to each other. Let us for the time being focus our attention on one of these subensembles, formed by a system consisting of two subsystems of $P < N$ and $N - P < N$ particles which behave locally to each other. Without loss of generality we can take $P \geq N - P$. Assume also for the time being that the first subsystem is formed by particles $1, 2, \ldots, P$ and the other by the remaining. We express our locality hypothesis of partial factorisability by assuming a factorisable expression for the probability $p(a_1 a_2 \cdots a_N)$ for observing the results a_i, for the observables $A^{(i)}$:

$$p(a_1 a_2 \cdots a_N) = \int q(a_1 \cdots a_P|\lambda) r(a_{P+1} \cdots a_N|\lambda)\, d\rho(\lambda) \tag{4.86}$$

where q and r are probabilities conditioned to the hidden variable λ with probability measure $d\rho$. Formulas similar to (4.86) with different choices of the composing particles and different value of P describe the other subensembles. We need not consider decomposition into more than two subsystems as then any two can be considered jointly as parts of one subsystem still behaving locally with respect to the others.

Consider the expected value of the product of the observables in the original ensemble

$$E(A^{(1)} A^{(2)} \cdots A^{(N)}) = \langle A^{(1)} A^{(2)} \cdots A^{(N)} \rangle = \sum_J (-1)^{n(J)} p(J) \tag{4.87}$$

where J stands for an N-tuple $j_1, \ldots, j_N$ with $j_k = \pm 1$, $n(J)$ is the number of -1 values in J and $p(J)$ is the probability of achieving the indicated values of the observables. Using the locality hypothesis of Eq. (4.86) as a constraint one can now derive inequalities satisfied by the numbers $E(A^{(1)} A^{(2)} \cdots A^{(N)})$ when we introduce alternative dichotomous observables for each of the particles. Following

[27] In Ref.[13] by Collins *et al.*. a different and independent derivation of the same results has been obtained.

[23] we assume, for simplicity, that there are two alternative observables $A_1^{(i)}, A_2^{(i)}$, $i = 1, 2, \ldots, N$ for each particle and we seek inequalities of the form

$$\sum_I \sigma_I E(A_{i_1}^{(1)} \cdots A_{i_N}^{(N)}) \leq M. \tag{4.88}$$

where $I = (i_1, i_2, \ldots, i_N)$ indicates which alternative observable was chosen for each particle, and $\sigma_I = \pm 1$ is a sign for each N-tuple I. The general set of such inequalities that are derived under the hypothesis of partial separability are called the *Svetlichny inequalities*, in analogy to the so-called Bell-inequalities which were derived under the hypothesis of full separability.

What is the explicit form of these Svetlichny inequalities? In other words what does the sequence σ_I look like? As the only permutation invariant of I is $t(I)$, the number of times index 2 appears in I, we must have $\sigma_I = \nu_{t(I)}$ for some $(N+1)$-tuple ($\nu_0 = 1$ by convention) $\nu = (1, \nu_1, \nu_2, \ldots, \nu_N)$. We must now solve for the possible values of ν.

Svetlichny and I have proven in our article [93] that there are at least two solutions for ν. These solutions are the *alternating* solutions and are as follows:

$$\nu_k^{\pm} = (-1)^{\frac{k(k\pm 1)}{2}}. \tag{4.89}$$

They are valid for all P. These sequences have period four with cycles $(1, 1, -1, -1)$ and $(1, -1, -1, 1)$ respectively. From what was said before, the alternating solutions test for all factorisable situations. The problem of finding *all* solutions for arbitrary P is a very difficult combinatorial problem which has not been addressed.

Introduce now the operator

$$S_N^{\pm} = \sum_I \nu_{t(I)}^{\pm} A_{i_1}^{(1)} \cdots A_{i_N}^{(N)}. \tag{4.90}$$

Using Eq. (4.88) the N-particle Svetlichny inequalities that arise from the alternating solutions can be expressed as

$$|\langle S_N^{\pm} \rangle| \leq 2^{N-1}. \tag{4.91}$$

For N even the two Svetlichny inequalities are interchanged by a global change of labels 1 and 2. For N odd, this is not the case. Consider the effect of such a change upon the cycle $(1, -1, -1, 1)$. If N is even, we get $(-1)^{N/2}(1, 1, -1, -1)$ which gives the second Svetlichny inequality. For N odd, we get $\pm(1, -1, -1, 1)$, which results in the same inequality. Similar results hold for the other cycle.

The two alternating solutions for $N = 2$ are the usual Bell-inequalities, the ones for $N = 3$ give rise to the two inequalities found in Eqs. (4.81, 4.82), and for $N = 4$ we have

$$\begin{aligned}
&|E(1111) + E(2111) + E(1211) + E(1121) + \\
&E(1112) - E(2211) - E(2121) - E(2112) - \\
&E(1221) - E(1212) - E(1122) - E(2221) - \\
&E(2212) - E(2122) - E(1222) + E(2222)| \leq 8,
\end{aligned}$$

where $E(1121)$ stands for $E(A_1^{(1)}A_1^{(2)}A_2^{(3)}A_1^{(4)})$ and similarly for all others. The second inequality is found by interchanging the observable labels 1 and 2. For arbitrary N the Svetlichny inequalities can be generated using either the two mentioned cycles for $\nu_k^{\pm}$ or some recursive relations which can be found in the next subsection. The logical result of the above is:

- Partial local HV-theory $\Longrightarrow$ Svetlichny inequalities.

These inequalities are a necessary condition for *any* PLHV theory to hold. One could conjecture that complete sets that are both necessary and sufficient could be generated but this conjecture is still under investigation[28].

Svetlichny Inequalities as a Sufficient Condition for N-partite Entanglement

The derivation of the N-partite Svetlichny inequalities is here supplemented with an application of the results to N-partite (entangled) quantum systems. The reason for this application is the recent experimental interest in quantum correlations in 3- and 4-particle systems [85, 89, 90, 91] (and the probable extension to even larger number of particles) where it becomes relevant to determine whether such correlations exhibit full N-particle quantum behavior and not just classical combinations of quantum behavior of a smaller number of particles.

The three-particle Svetlichny inequalities gave sufficient tests for full three-particle entanglement. Does the same also hold for the N-particle case? Yes, indeed. The partial factorisability analysis leading to the Svetlichny inequalities provides experimentally accessible sufficient conditions for full N-partite entanglement, i.e. conditions to distinguish between N-particle states in which all N particles are entangled to each other and states in which only P particles are entangled (with $P < N$). The inequalities that provide these sufficient conditions will be here also shown to be maximally violated by the N-partite GHZ-states. However, before presenting these results I would like to investigate N-partite entanglement a little further.

I will address the general question of whether correlations in N-partite quantum behavior exhibit true N-partite entanglement and not just classical combinations of quantum behavior of a smaller number of bodies. In other words, what N-partite QM-states (pure and mixed) are nonlocal in the sense that they do not allow for certain PLHV-models, and furthermore, what sufficient and/or necessary conditions for true N-particle entanglement are involved?

N-particle entanglement is fundamentally different from the well-studied two particle entanglement because not only is the classification of the entanglement a problem [52] it also requires different necessary and sufficient conditions for actual experimental proof. In the case of two particle entangled states it is sufficient to show that the observed data cannot be explained in a local realist way. That is, it is sufficient for the correlations between the observed data to violate a certain Bell-type inequality [60] because all two-particle entangled states can be made to violate such a Bell-inequality [42]. However, in the case of experimental proof of N-particle entanglement is is not sufficient to show that the observed data

[28] G.Svetlichny; private communication.

violates a standard generalized N-particle Bell-inequality such as for example derived by Mermin [29] and Ardehali[43]. These N-particle generalizations of the Bell-type inequality assume full factorisability, i.e. they treat all particles as unentangled in the sense that they can be assigned independent elements of reality for certain measurement outcomes. Certain bounds on correlations of expectation values are then derived and are then shown to be violated by the corresponding quantum mechanical expectation values by a maximal factor that grows exponentially with N [29, 43]. N-particle experiments that violate these inequalities are then proofs of some sort of non-locality in quantum mechanics that contradicts the assumptions of local realism. More explicitly, it would then be shown that no completely factorisable probability distribution can account for the observed data.

However, the violation of local realism for full factorisability is not sufficient for confirmation of entanglement of all N particles. The question if some observed state admits a model with any form of factorisability, not only full factorisability for all particles must be addressed. The standard generalized Bell-type inequalities to test local realism are not able to distinguish between mixtures of less than N-particle entangled states and the maximal entangled state in which all N particles are entangled. All they show is that the observed data exhibits some 'non-local' correlations, i.e. some entanglement. To show full N-particle entanglement, other conditions than merely violating a generalized Bell-type inequality are needed. We have already seen such conditions. For bi-partite states the Bell-inequality itself was shown to be such a sufficient condition. Further, the Bell-Klyshko inequality was turned into such a condition for full N-partite entanglement in Eq.(4.78) and also the fidelity measure of section 3.2.5 is such a condition. However, below I will present another of such a condition using the Svetlichny inequalities. In chapter 5 this condition and the condition derived from the fidelity measure will be explicitly compared to each other.

Let's go back to the N-particle Svetlichny inequalities of Eq.(4.91) as given in the last subsection. They were derived for hidden variable states λ. However, as Svetlichny and I have shown, they also hold for N-partite quantum states which are $(N-1)$ partite entangled (or non-entangled). In order to see this, suppose we choose the set of all hidden variables to be the set of all states on the Hilbert space $\mathcal{H}$ of the system and $\rho(\lambda) = \delta(\lambda - \lambda_0)$ where λ_0 is a quantum state in which one particle (say the N-th) is independent from the others, i.e.:

$$\rho = \rho^{\{1,\dots,N-1\}} \otimes \rho^{\{N\}}. \tag{4.92}$$

We then recover the factorisable condition of Eq.(4.86):

$$p(a_1 a_2 \cdots a_N|\lambda_0) = p_{\rho^{\{1,\dots,N-1\}}}(a_1 a_2 \cdots a_{N-1}) p_{\rho^{\{N\}}}(a_N) \tag{4.93}$$

where $p_{\rho^{\{1,\dots,N-1\}}}(a_1 a_2 \cdots a_{N-1})$ and $p_{\rho^{\{N\}}}(a_N))$ are the corresponding (joint) quantum mechanical probabilities to obtain $a_1, a_2, \cdots, a_N$ for measurements of observables $A^{(1)}, A^{(2)}, \cdots, A^{(N)}$. The expectation value $E(A^{(1)}A^{(2)}\cdots A^{(N)})$ then becomes the quantum mechanical expression: $E_{\lambda_0}(A^{(1)}A^{(2)}\cdots A^{(N)}) = \mathrm{Tr}[\rho^{\{1,\dots,N-1\}} A^{(1)} \otimes A^{(2)} \otimes \cdots \otimes A^{(N-1)}]\mathrm{Tr}[\rho^{\{N\}} A^{(N)}]$. Thus the same bound as in the Svetlichny inequalities of Eq.(4.91) holds also for the quantum mechanical expectation values for a state of the form Eq.(4.92).

Since the Svetlichny inequalities of Eq.(4.91) are invariant under a permutation of the N particles, this bound holds also for a state in which another particle than the N-th factorises, and, since the inequalities are convex as a function of ρ, it holds also for mixtures of such states. Hence, for every $(N-1)$-particle entangled state ρ we have

$$|\langle S_N^{\pm}\rangle_\rho| = |\mathrm{Tr}(\rho S_N^{\pm})| \leq 2^{N-1}. \tag{4.94}$$

Thus, a sufficient condition for full N-particle entanglement is a violation of Eq.(4.94). States that indeed violate these N-partite Svetlichny inequalities I will call *Svetlichny correlated states.*

The logical result of the above is as follows:

- $\neg$ full entanglement = partial/full separability $\Longrightarrow$ non-violation of Svetlichny inequalities.

And consequently the following holds as well:

- $\neg$ full entanglement = Partial/full separability $\Longrightarrow$ partial local HV-theory holds.

The maximal quantum mechanical violation for the left-hand side of the N-particle Svetlichny inequalities of Eq.(4.91) is obtained for fully entangled N-particle quantum states and is equal to $2^{N-1}\sqrt{2}$. To see this note that the following recurrence relations hold[29].

$$S_N^{\pm} = S_{N-1}^{\pm} A_1^{(N)} \mp S_{N-1}^{\mp} A_2^{(N)}. \tag{4.95}$$

Consider the term $S_{N-1}^{\pm} A_1^{(N)}$ which is a self-adjoint operator. The maximum K of the modulus of its quantum expectation $|\langle S_{N-1}^{\pm} A_1^{(N)}\rangle|$ is equal to the maximum modulus of its eigenvalues. The two factors commute (they act on different tensor factors) and are self-adjoint. The eigenvalues of the product is the product of the eigenvalues of the factors. Since the eigenvalues of $A_1^{(N)}$ are ± 1, we see that K is equal to the maximum of $|\langle S_{N-1}^{\pm}\rangle|$. Similarly for the other term. Thus one can take the N-particle bound as twice the $(N-1)$-particle bound. Since the bound on the Bell-inequality is $2\sqrt{2}$ [17] the result follows.

This upper bound is in fact achieved for the Greenberger-Horne-Zeilinger (GHZ) states for appropriate values of the polarizer angles of the relevant spin observables. These states thus are examples of Svetlichny-correlated states. To see this consider the general GHZ state:

$$\Psi_N = \frac{1}{\sqrt{2}}(|\uparrow\rangle^{\otimes N} \pm |\downarrow\rangle^{\otimes N}) = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\cdots\uparrow\uparrow\rangle \pm |\downarrow\downarrow\cdots\downarrow\downarrow\rangle).$$

Let $A_i^{(k)} = \cos\alpha_i^{(k)}\sigma_x + \sin\alpha_i^{(k)}\sigma_y$denote spin observables with angle $\alpha_i^{(k)}$ in the x-y plane. A simple calculation shows

$$E(i_1\cdots i_N) = \pm\cos(\alpha_{i_1}^{(1)} + \cdots + \alpha_{i_N}^{(N)}) \tag{4.96}$$

[29] The recurrence relations of Eq.(4.95) are an important result. It is a starting point for future research. For example Uffink [11] uses them to make the extension to *quadratic* inequalities that provide stronger sufficient conditions for full N-partite entanglement than both the Bell-Klyshko inequality and the Svetlichny inequality.

where the sign is the sign chosen in the GHZ state.

We now note that for $k = 0, 1, 2, \ldots$ one has: $\cos\left(\pm\frac{\pi}{4} - k\frac{\pi}{2}\right) = \nu_k^{\pm}\frac{\sqrt{2}}{2}$ where $\nu_k^{\pm}$ is given by (4.89). This means that by a proper choice of angles, we can match, up to an overall sign, the sign of the cosine in Eq.(4.96) with the sign in front of $E(i_1 \cdots i_N)$ as it appears in the inequality, forcing the left-hand side of the inequality to be equal to the maximum value $2^{N-1}\sqrt{2}$. This can be easily done if each time an index i_j changes from 1 to 2, the argument of the cosine is decreased by $\frac{\pi}{2}$. Choose therefore

$$\begin{aligned}\left(\alpha_1^{(1)}, \alpha_1^{(2)}, \ldots, \alpha_1^{(N)}\right) &= \left(\pm\frac{\pi}{4}, 0, \ldots, 0\right)\\ \left(\alpha_2^{(1)}, \alpha_2^{(2)}, \ldots, \alpha_2^{(N)}\right) &= \left(\pm\frac{\pi}{4} - \frac{\pi}{2}, -\frac{\pi}{2}, \ldots, -\frac{\pi}{2}\right)\end{aligned}$$

where the sign indicates which of the two $\nu^{\pm}$ inequalities is used. This specification of the angles will result in the upper bound.

4.5 Dual Purpose of Bell-type inequalities

Bell-type inequalities were derived as necessary conditions for certain HV-theories, but they were also seen to result in sufficient conditions for full bi-partite and multi-partite entanglement. Thus these inequalities serve a dual purpose:

Purpose (A) Bell-type inequalities as tests for local HV-theories.

Purpose (B) Bell-type inequalities as tests for (full) multi-partite entanglement.

I will now recall both these purposes in detail using a formulation that was inspired by Jos Uffink. However, I first need to define some terminology.

- BI = Bell-Inequality: $|E^{lr}(\mathcal{B})| \leq 2$. See further definition in Eq.(4.24) of section 4.2.5.
- BK = Bell-Klyshko Inequality: $|E^{lr}(F_N)| \leq 2^{N/2}$. See further definition in Eq.(4.75) of section 4.4.1.
- SI = Svetlichny Inequality: $|E^{lr}(S_N^{\pm})| \leq 2^{N-1}$. See further definition in Eq.(4.94) of section 4.4.2.
- S_N^M = The set of $N - M$ partite entangled N-partite states, with $M < N$, and all lesser entangled states. See section 3.2.3 for the definition of these states.
- S_N = The total set of N-partite quantum states, thus also including full entanglement. See section 3.2.3 for the definition of these states.

Using this terminology I will present the results so far obtained for both purpose (A) and (B).

Bi-partite entanglement and local HV-theory.

- Purpose (A)

$$\text{local HV} \Longrightarrow \text{BI}$$
$$\text{QM} \Longrightarrow \neg\ \text{BI}$$

- Purpose (B)

$$\rho \in S_2^1 : \qquad |E_\rho(\hat{\mathcal{B}})| \leq 2$$
$$\rho \in S_2 : \qquad |E_\rho(\hat{\mathcal{B}})| \leq 2\sqrt{2}$$

N-partite entanglement and local HV-theory.

- Purpose (A)

$$\text{local HV} \Longrightarrow \text{BK}$$
$$\text{QM} \Longrightarrow \neg\ \text{BK}$$

- Purpose (B)

$$\rho \in S_N^1 : \qquad |E_\rho(\hat{F}_N)| \leq 2$$
$$\rho \in S_N^{N-1} : \qquad |E_\rho(\hat{F}_N)| \leq 2^{N/2}$$
$$\rho \in S_N : \qquad |E_\rho(\hat{F}_N)| \leq 2^{N/2}\sqrt{2}$$

N-partite entanglement and partial local HV-theory.

- Purpose (A)

$$\text{Partial local HV} \Longrightarrow \text{SI}$$
$$\text{QM} \Longrightarrow \neg\ \text{SI}$$

- Purpose (B)

$$\rho \in S_N^{N-1} : \qquad |E_\rho(\hat{S}_N^{\pm})| \leq 2^{N-1}$$
$$\rho \in S_N : \qquad |E_\rho(\hat{S}_N^{\pm})| \leq 2^{(N-1)}\sqrt{2}$$

In all three cases, in purpose (B) the maximum bound for the quantum case can indeed be obtained using the generalized GHZ states $\left|\psi_{\text{GHZ}}^N\right\rangle$.

4.6 Classification of Quantum States. Part III. Classification through Factorisability and HV-simulability

The confrontation in this chapter of the hidden variables program and the doctrine of local realism with the structure of the quantum mechanical state space, has led to the identification and classification of some special quantum states. This is only a preliminary fraction of such a classification. In the next chapter this will be extended when results of this chapter are explicitly compared to results of the previous chapter about separability and distillability of quantum states. However, let me first present the special states that have been distinguished so far through factorisability and HV-simulability.

- **Bell-correlated states.** Bi-partite quantum states that can be made to violate the CHSH inequality. In section 4.2.5 we see a first set of such states, i.e the bi-partite singlet states. But in the next chapter the full set will be explored.

- **Hardy-states.** Quantum states that can produce a Hardy type argument. On such a set of Hardy states are the bi-partite states of Eq.(4.57) in section 4.3.2.

- **Svetlichny-correlated states.** In analogy to the Bell-correlated states, the Svetlichny-correlated states are N-partite states that can be made to violate the generalized Svetlichny inequalities of Eq.(4.91) of section 4.4.2. As shown in this section, the set of N-partite GHZ-states is an examples of such states.

4.7 Conclusion and Summary

This chapter started with the incompleteness problem of quantum mechanics. This problem, whether or not quantum mechanics provides a complete physical theory, has led to the study of hidden variable theories since they could possibly provide more complete theories than QM itself. The structure of these hidden variable theories has been presented in a somewhat historical setting. Here we have seen that the initial requirement of non-contextuality of these HV-theories was changed into the physical requirement of locality. Subsequently the doctrine of local realism was defined as a local hidden variable theory that has to meet the quantum criterium. Then, the question whether a local HV-theory could exist for QM was shown to be answered in the negative by John Bell. He derived the nowadays called Bell-inequalities necessary for any HV-theory and showed that QM would violate these inequalities. This is the content of the Bell-theorem.

The derivation of the Bell-inequalities and the Bell-theorem itself were presented as preliminary work for the remainder of this chapter. In this remainder more complex systems were studied than the bi-partite spin-1/2 systems which were the paradigmatic systems for the original Bell-theorem and all its initial variations on the same theme.

In section 4.3 more complex bi- and tri-partite systems were considered leading to new *Gedankenexperiments*, the so-called Bell-theorems without inequalities and the algebraic theorems. As examples the Bell-theorem without inequalities of Hardy and the algebraic proof of GHZ have been discussed. These new Bell-theorems are compared to the original Bell-theorem for logical strength and experimental testability. The algebraic Bell-theorem of GHZ has been argued to be the logically most strong theorem. It requires a minimum of quantum structure to arrive at a contradiction with local realism. However, from an experimental point of view the original Bell-theorem has been argued to be superior because it can be most easily experimentally implemented. The Bell-theorem without inequalities of Hardy and the algebraic proof of GHZ were in fact argued to break down because of neglect of measurement compatibility.

The extension to N-partite systems has resulted in the necessary distinction between the specific locality-hypotheses of full and partial factorisability. The

Bell-Klyshko N-partite Bell-type inequalities for full factorisability were presented and furthermore they were extended to complete sets (i.e. necessary and sufficient sets) of Bell-type inequalities for local realism to hold. The extension to multi-partite systems for which the specific locality hypothesis of partial factorisability is required to hold, has been shown to ask for a new type of hidden variable theories, the so-called Partial Local Hidden Variable Theories. The generalized Svetlichny inequalities were derived and they were shown to be necessary inequalities for any PLHV to hold.

The three types of inequalities – the Bell-inequalities, the N-partite Bell-Klyshko inequalities for full separability and the Svetlichny inequalities for partial separability – were all confronted with the structure of the quantum mechanical state space. As a result we have seen that these inequalities give sufficient conditions for respectively bi-partite and full N-partite entanglement. These inequalities thus serve a dual purpose. As tests for the possibility of certain HV-models and as tests for entanglement. This was presented in section 4.5.

Finally, the confrontation with the structure of the quantum mechanical state space has led to an extension of the two quantum state classifications of the previous two chapters. A classification through factorisability and HV-simulability was presented in the last section of this chapter.

Chapter 5

Quantum Mechanics vs. Local Hidden Variable Theories.

5.1 Introduction

We have already seen one confrontation of quantum mechanics with the hidden variable structure of chapter 3. This was presented in the last chapter in section 4.5 and dealt with the following: The three types of inequalities – the Bell-inequalities, the N-particle Bell-Klyshko inequalities for full separability and the Svetlichny inequalities for partial separability – were derived as necessary conditions for certain HV-theories, but they were also seen to result in sufficient conditions for bi-particle and full multi-particle entanglement. Thus these inequalities serve a dual purpose: as tests for the possibility of certain HV-models and as tests for entanglement. In these results two different aspects of the Bell-type inequalities are used. The first is related to (partial) local hidden variable theories and the question of whether or not they exist for quantum mechanical predictions. The second is related to the entanglement structure of quantum mechanics. These two aspects will be further explored.

Section 5.2.1 and 5.2.2 deal respectively with the quantum mechanical violations and non-violations of the Bell-type inequalities of the previous chapter for full factorisability. This leads to a classification of entanglement and separability, i.e. specific states violating and not violating Bell-type inequalities for specific measurement configurations. In section 5.3 the results about the relationship of the quantum mechanical state space with the hidden variable structure for the case of full factorisability are presented in implication diagrams. The extension to partial factorisability and the corresponding Svetlichny inequalities and partial local HV-theories will be performed in section 5.4. Here the known quantum mechanical violations and non-violations of the Svetlichny inequalities are presented. In section 5.5 all results obtained about the relationship of the quantum mechanical state space with the hidden variable structure for case of partial factorisability, will be presented in implication diagrams. In order to continue the classification of the quantum state space, the newly distinguished quantum states of this chapter are summarized in section 5.6. This chapter ends with a discussion in section 5.7.

5.2 Quantum Mechanical (Non-)Violations of the Bell-inequalities.

5.2.1 Violations

We have seen some quantum mechanical violations of the Bell-type inequalities of chapter 3 However, only some specific states were considered and no systematic study was performed to find all states that can violate a specific Bell-inequality. In this section such a study will be performed. Specific question are:

- What is the set of Bell-correlated states, i.e. violating a Bell-type inequality?
- What states would violate the different inequalities maximally?

To answer these questions some distinctions have to be made to exactly specify the type of systems and the type of inequalities that one is dealing with. These distinctions are[58]:

1. Types of Systems.
   (a) The number of subsystems (particles) M.
   (b) The dimension $dim\mathcal{H}$ of the Hilbert space per particle.
2. Types of Inequalities, i.e. measurement configurations (N,m,d).
   (a) The number N of systems being measured.
   (b) The number of observables m that is being measured on each particle.
   (c) The number of different outcomes d per observable. (d-valued observables.)

These two types are related since $N \leq M$ and $d \leq \dim\mathcal{H}$. For each of these types of systems and types of inequalities I will now present the known Bell-type inequalities that test local HV-theories for the relevant measurement configurations, as well as the known results for quantum violations of these inequalities.

Bi-particle

- $dim\mathcal{H} = 2$.
  - **Measurement configuration (2,2,2), i.e. two dichotomous observables per site.**
    As we have seen the measurement configuration $(2, 2, 2)$ gives rise to the CHSH-inequality $|E^{lr}(\mathcal{B})| \leq 2$ with $\mathcal{B}$ the Bell-polynomial of Eq. (4.21). The best upper bound for violation of this inequality using

quantum states, $|E_\rho(\hat{\mathcal{B}})| \leq 2\sqrt{2}$, is first derived by Cirelson [17]. He used the square of the Bell operator and the variance inequality

$$\text{Tr}[\rho\hat{\mathcal{B}}]^2 \leq \text{Tr}[\rho\hat{\mathcal{B}}^2]. \tag{5.1}$$

Because the observables are all unitary one gets:

$$\hat{\mathcal{B}}^2 = 4\mathbb{1} - [\hat{A}_1, \hat{A}_2] \otimes [\hat{B}_1, \hat{B}_2]. \tag{5.2}$$

These commutators are bounded as follows: $\|[\hat{A}_1, \hat{A}_2]\| \leq 2\|\hat{A}_1\| \; \|\hat{A}_2\|$ and thus $\|\hat{\mathcal{B}}^2\| \leq 8$. Taking the square root one gets the so-called *Cirelson bound* on the CHSH-inequality:

$$\text{Tr}[\hat{\mathcal{B}}\rho] \leq 2\sqrt{2}. \tag{5.3}$$

This is also called *Cirelson's inequality*. It holds for all bi-particle quantum systems and measurement configurations $(2,2,2)$. In section 4.2.5 we have seen that the singlet state gives this maximal bound. Furthermore in section 4.2.6 it was shown that violation of the CHSH inequality provides a sufficient condition for bi-particle entanglement for systems with $dim\mathcal{H} = 2$.

– **Maximum violation for bi-particle two-dimensional systems**

What other states besides the singlet state maximally violate the CHSH inequality? Does it have to be a pure state? Aravind [5] and the Horodecki's [62] investigated these questions by calculating the extent to which mixed states can maximally violate the CHSH inequalities.

I will here present the method used by the Horodecki's. Consider a quantum state ρ of two bi-particle two-dimensional systems. For these systems it is sufficient to consider only observables of the form $\hat{A}_k = \vec{a_k}\vec{\sigma}$, where $\vec{\sigma}$ is the Pauli vector and $\vec{a_k}$ a normalised vector in $\mathbb{R}^3$. The maximum value is found by maximizing $\text{Tr}[\rho\hat{\mathcal{B}}]$ with respect to $\vec{a_1}, \vec{a_1}', \vec{a_2}, \vec{a_2}'$, i.e. the maximum is taken over all unit vectors.

Consider an arbitrary two-level two particle state ρ. Define the matrix $T_{ij} = \text{Tr}(\rho\sigma_i \otimes \sigma_j)$. The Horodecki's then show that the maximal violation of the CHSH inequality is given by:

$$\begin{aligned}
\text{Tr}[\rho\hat{\mathcal{B}}]_{max} &= \max_{\vec{a_1},\vec{a_1'},\vec{a_2},\vec{a_2'}} (\vec{a_1}\cdot T(\vec{a_2}+\vec{a_2}') + \vec{a_1}'\cdot T(\vec{a_2}-\vec{a_2}')) \\
&= \max_{\vec{a_2},\vec{a_2}'} (\| T(\vec{a_2}+\vec{a_2}') \| + \| T(\vec{a_2}-\vec{a_2}') \|) \\
&= \max_{\phi,\vec{c}\perp\vec{c'}} \cos\phi \, \| T\vec{c} \| + \sin\phi \, \| T\vec{c'} \| \\
&= \max_{\vec{c}\perp\vec{c'}} \sqrt{\| T\vec{c} \|^2 + \| T\vec{c'} \|^2}.
\end{aligned} \tag{5.4}$$

This last maximum gives

$$\text{Tr}[\rho\hat{\mathcal{B}}]_{max} = \sqrt{\gamma + \gamma'}, \tag{5.5}$$

where γ, γ' are the two largest eigenvalues of the matrix $T^T T$. For pure states –for which there always is a bi-orthonormal basis $\{ |0\rangle, |1\rangle \}$ so that they can be written in Schmidt form as $|\psi\rangle = \cos\phi\,|00\rangle + \sin\phi\,|11\rangle$– this becomes:

$$\mathrm{Tr}[\rho\hat{\mathcal{B}}]_{max} = 2\sqrt{1+\sin^2(2\phi)}. \tag{5.6}$$

From this result we see two implications. First, as soon as a pure state becomes entangled ($\phi \neq n\pi/2,\ n = 1, 2, \dots$) it violates a Bell inequality. Second, the maximum violations are achieved for the states for which $\cos\phi = \sin\phi$, i.e. for states that can be written in the special Schmidt form with equal Schmidt coefficients: $|\Psi\rangle = \frac{\pm 1}{\sqrt{2}}(|00\rangle \pm |11\rangle)$. This last implication is the motivation for using the term *maximally* in the definition of maximally entangled states in section 3.2.1[1].

– **Measurement configuration** $(2, m, 2)$**, i.e.** m **dichotomous observables per site.**

So far only two different observables at each site were chosen in the construction of the inequalities. Gisin [103] however has presented a generalization to arbitrary many observables. I will now present the results of the method of Gisin to construct inequalities for bi-particle systems with m dichotomous observables measured at each system, i.e. for the measurement configuration $(2, m, 2)$.

Consider observables A_i and B_i with outcomes $a_i = \pm 1$ and $b_i = \pm 1$ for $i = 1, \dots, m$. The local realistic expectation value for observing A_i and B_j on each of the subsystems are as usual denoted by the factorisable condition $E^{lr}(A_i, B_j) = \int d\lambda M(\lambda) a(A_i, \lambda) b(B_j, \lambda)$, where $a(A_i, \lambda) = \pm 1$ is the outcome of the observation of A_i for the system in the state λ and similarly for $b(B_j, \lambda) = \pm 1$. Gisin obtained the following inequality for the expectation values for the m different observables:

$$\begin{aligned} G(m) &= \sum_{i=1}^{m}\Big(\sum_{j=1}^{m+1-i} E^{lr}(A_i, B_j) - \sum_{k=m+2-j}^{m} E^{lr}(A_i, B_k)\Big) \\ &\leq \left[\frac{m^2+1}{2}\right] \equiv G_{lr}(m), \end{aligned} \tag{5.8}$$

where $[x]$ is the largest integer smaller or equal to x. For $m = 2$ this is the usual CHSH-inequality.

Gisin argues that the maximal violation using quantum states is obtained with the maximally entangled states and gives the value

$$G_{QM}(m) = \frac{2m\cos(\pi/2m)}{\sin(\pi/m)} > \left[\frac{m^2+1}{2}\right] = G_{lr}(m). \tag{5.9}$$

[1]Recall this definition: Two N level systems A and B are called *maximally entangled* when their composed state $|\Psi\rangle$ in the Schmidt decomposition can be written as

$$|\Psi\rangle = \frac{1}{\sqrt{N}}\sum_{i=0}^{i=N} |\phi_i\rangle \otimes |\psi_i\rangle \tag{5.7}$$

with $\{|\phi_i\rangle^A\}$ and $\{|\psi_i\rangle^B\}$ two orthonormal bases on $\mathcal{H}^A$ and $\mathcal{H}^B$ with dimension d_A and d_B.

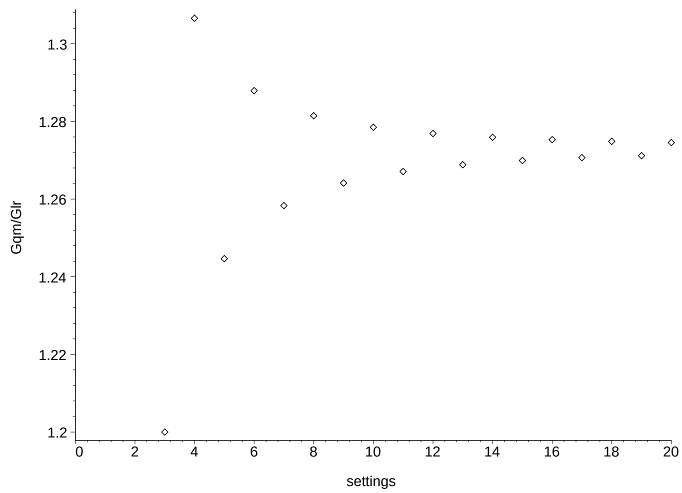


Figure 5.1: $\frac{G_{QM}(m)}{G_{lr}(m)}$ as a function of the number of settings m.

However Gisin gives no proof of this maximal violation and it could very well be that other states give larger violations. He has shown that for large m the ratio of violation becomes:

$$\frac{G_{QM}(\infty)}{G_{lr}(\infty)} = \lim_{m\to\infty} \frac{2m\cos\pi/2m}{\sin\pi/m} \Big/ \left[\frac{m^2+1}{2}\right] = \frac{4}{\pi} \approx 1.27. \qquad (5.10)$$

See figure 5.1. It is interesting note that the ratio of violation asymptotically tends to $4/\pi$ as m grows.

- *dim*$\mathcal{H}$ **arbitrary.**
  - **Measurement configuration** $(2,2,2)$**.**

In the previous cases the subsystems were two dimensional. Gisin and Peres [96] have considered the extension to any *dim*$\mathcal{H}$ for pure states. They show that for *any* pure entangled state of two quantum systems, it is possible to find observables whose correlations violate the CHSH inequality. Because the systems can have in general any dimension, one could in principle use observables corresponding to self-adjoint operators with as many possible outcomes as there are dimensions. However, Gisin and Peres construct for each possible system two dichotomous observables. In effect they thus consider the measurement configuration $(2,2,2)$ and the problem they solve is finding observables that allow for violation of the local realistic inequalities that hold for this measurement configuration. These are in fact the CHSH-inequalities.

I will not give the proof, but will only present the ideas behind it. Make use of the fact that any bi-particle pure state $|\,\psi\rangle$ on $\mathcal{H}_1\otimes\mathcal{H}_2$, each with dimension equal to H, can be written as a Schmidt bi-orthogonal sum

$$|\psi\rangle = \sum_i^H c_i \,|\phi\rangle_i \otimes |\chi\rangle_i \tag{5.11}$$

where $\{|\phi\rangle_i\}$ and $\{|\chi\rangle_i\}$ are orthonormal bases in $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively. Gisin and Peres then restrict their attention to the w-dimensional subspaces of $\mathcal{H}_1 \otimes \mathcal{H}_2$ that corresponds to non-vanishing c_i. Only the case $w > 1$ is considered because this corresponds to the entangled states. For these states they construct specific dichotomous observables such that the CHSH-inequality is violated. The maximal extent of this violation has not been investigated.

– **General measurement configuration** $(2, m, K)$**.**

The most general inequalities for bi-particle systems with two K-dimensional subsystems correspond to the measurement configuration $(2, m, K)$ that considers m K-valued observables per subsystem. However as far as I know no results have been obtained for this general case.

N-particle

- $dim\mathcal{H} = 2$

– **Measurement configuration** $(N, 2, 2)$

The most simple extension from two to N particles is the extension of the CHSH inequalities to N-parties, i.e. the extension to the measurement configuration $(N, 2, 2)$. As mentioned before in section 4.4.1 Mermin [29] was the first to obtain such inequalities. These inequalities were shown to be violated by quantum mechanics with a factor exponentially growing with N. In fact for N even the ratio of violation is equal to $2^{(N-2)/2}$ and for N odd it is $2^{(N-1)/2}$. Ardehali [43] derived a similar set of N-particle inequalities with the results for N odd and N even interchanged. Using a complicated inequality Roy and Singh [7] obtained the result that for any N the ratio of violation is equal to $2^{(N-1)/2}$.

To get a feeling of how these first generalized inequalities were derived I will discuss the original Mermin inequality. He considered the N-particle GHZ state $\left|\psi^N_{\mathrm{GHZ}}\right\rangle = (|\uparrow\uparrow\ldots\rangle + i\,|\downarrow\downarrow\rangle\ldots)/\sqrt{2}$ and the following operator:

$$\hat{\mathcal{A}} = \frac{1}{2i}\Big(\prod_{k=1}^{N}(\sigma_{x_k} + i\sigma_{y_k}) - \prod_{k=1}^{N}(\sigma_{x_k} - i\sigma_{y_k})\Big). \tag{5.12}$$

This is a generalization of the Bell-operator $\hat{\mathcal{B}}$. It follows that the expectation value of this operator, denoted as E^{QM}, is equal to:

$$E^{QM}(\hat{\mathcal{A}}) = \langle\,\psi|\,\hat{\mathcal{A}}\,|\,\psi\rangle = 2^{N-1}. \tag{5.13}$$

However its local realistic value assuming factorisability for the expectation values of products of observables is equal to:

$$E^{lr}(A) = \int d\lambda M(\lambda)\frac{1}{2i}\Big(\prod_{k=1}^{N}(E^{lr}_{x_k}(\lambda)S + iE^{lr}_{y_k}(\lambda)) - \prod_{k=1}^{N}(E^{lr}_{x_k}(\lambda) - iE^{lr}_{y_k}(\lambda))\Big), \quad (5.14)$$

where $M(\lambda)$ is the hidden variable distribution and $E^{lr}_x(\lambda)$, $E^{lr}_y(\lambda)$ are the expectation values determined by the local HV-theory in the hidden variable state λ for the local measurements of the spin in the x- and y-direction.

The value of E^{lr} was shown by Mermin to be bounded as follows:

$$E^{lr}(A) \leq 2^{(N-\alpha)/2}, \quad (5.15)$$

with $\alpha = 0, 1$ for N even and N odd respectively. Comparing this to the value obtained by the GHZ-states we see that a ratio of violation is obtained that grows exponentially with N.

The original Mermin inequality was succeeded by similar ones derived by Ardehali, Roy and Singh. These were further generalized by Klyshko and Belinsky [10, 98] and Gisin and Bechmann-Pasquinucci [97] and were already presented in section 4.4.1.

Finally, as was shown in the previous chapter, section 4.4.1, complete sets of inequalities exist for this measurement configuration.

- **General measurement configurations** $(N, m, 2)$

  The most general inequalities for N-particle systems with two-dimensional subsystems correspond to the measurement configuration $(N, m, 2)$ that considers m bi-valued observables per subsystem. However as far as I know no results have been obtained for this general case.

• $dim\mathcal{H}$ **arbitrary.**

- **Reduction to measurement configuration** $(2, 2, 2)$

  So far we have only seen $dim\mathcal{H} = 2$ for each of the N particles. The extension to any dimension has first been performed by Popescu and Rohrlich [9]. They cleverly consider a method that circumvents the difficult task to find inequalities for the measurement configuration $(N, 2, K)$ In effect they reduce the problem to the $(2, 2, 2)$-case.

  For every N-particle pure state where each of the particles has arbitrary dimension greater than or equal to, two inequalities are given, not for the difficult measurement configuration $(N, 2, K)$, but for the more simple measurement configuration $(2, 2, 2)$. In fact the well known CHSH-inequalities are used. In essence Popescu and Rohrlich prove that for every pure entangled state (N-particle, arbitrary dimension) a measurement procedure and a set of observables can be found such that for these states and for specific dichotomous observables the CHSH inequality is violated.

The method used is to consider projections of the original quantum state using local observables onto a direct product of subspaces such that the resulting bi-particle state is still entangled. In other words, they prove that for any pure entangled N-particle state, for any two of the N-systems, there exists a projection onto a direct product of states of the other $N-2$ systems, that leaves the two systems in an entangled state [9].

Because the projection is onto a direct product of states it suffices to consider only local measurements and still the remaining entangled bi-particle state can be made to violate the CHSH-inequality. Thus by conditioning the quantum mechanical predictions for two systems on a particular outcome $c_k, d_l, \ldots$ of local measurements of the other $N-2$ systems, the CHSH inequality

$$|E(\hat{A},\hat{B},c_k,d_l,\ldots)+E(\hat{A},\hat{B}',c_k,d_l,\ldots)+ \\ E(\hat{A}',\hat{B},c_k,d_l,\ldots)-E(\hat{A}',\hat{B}',c_k,d_l,\ldots)|\leq 2 \quad (5.16)$$

can be violated by measurements of the four specific observables $\hat{A}$, $\hat{A}'$, $\hat{B}$ and $\hat{B}'$ that Popescu and Rorhlich have proven to exist. This method can perhaps be considered the first distillation protocol.

– **Measurement configuration (N,2,K)**

Home and Majumbar [8] consider N spin j-systems (dimension $K = 2j+1$) for which they derive an inequality for the measurement configuration $(N,2,2j+1)$ This inequality is the extension of the $(N,2,2)$-case derived by Mermin presented in the previous section. They use the same nonlocal observable $\hat{\mathcal{A}}$ as Mermin used in Eq.(5.12) but with the Pauli-operator σ_{μ_k} replaced by the spin-operator $\hat{S}_{\mu_k}$ with μ equal to x or y.

Again assuming factorisability for the expectation values of the spin observables one gets for the expectation value of $\hat{\mathcal{A}}$

$$F^{lr} \leq 2^{N/2} j^N, \quad (5.17)$$

for the local realist bound. For two spin-$\frac{1}{2}$ particles one gets $F^{lr} \leq 1/2$. (Note that whereas the Pauli operator has fixed eigenvalues ± 1, the maximal eigenvalues of $\hat{S}_{\mu_k}$ are equal to $j,\ 2j,\ 3j,\ldots$.) Using a specific entangled quantum state one gets

$$F^{QM}_{max} > 2^{N/2} j^N = F^{lr}_{max}, \quad (5.18)$$

which cannot be shown analytically –it means solving polynomial equations of quartic or higher degree– but has been shown numerically [8]. For two spin-$\frac{1}{2}$ particles one gets $F^{QM} = 2$. This quantum mechanical result is a factor 4 greater than the local realistic result. This

Table 5.1: Results of Home and Majumbar.

j	N	F_{max}^{QM}	F_{max}^{lr}	$F_{max}^{QM}/F_{max}^{lr}$
3/2	2	11	4.5	2.44
3/2	10	5.5×10^5	1.8×10^3	306
5/2	2	14.6	12.5	1.17
5/2	10	7.7×10^6	3.0×10^5	25.7
9/2	2	61	40.5	1.51
9/2	10	3.3×10^9	1.1×10^8	30.0
21/2	2	448	220.5	2.03
21/2	10	1.2×10^13	5.2×10^{11}	23.1

incompatibility between F_{max}^{lr} and F_{max}^{QM} persists both for growing N and for growing j. To get an impression of the quantitative values, I present the result for spin 3/2, 5/2, 9/2 and 21/2 for both $N = 2$ and $N = 10$ in table 5.1. Thus, on the basis of these numerical results Home and Majumbar have shown that the quantum mechanical expectation value of the specific operator of Eq.(5.12) (with σ_{μ_k} replaced by the spin-operator $\hat{S}_{\mu_k}$) exceeds the local realist bound and further that the violation grows for large N and persists for large j.

– **Most general measurement configuration** (N, m, K)**.**

The most general inequalities for N-particle systems with K-dimensional subsystems correspond to the measurement configuration (N, m, K) that considers m K-valued observables per subsystem. However as far as I know no results have been obtained for this most general case.

Macroscopic Divergence.

We have just seen that the numerical results in table 5.1 of Home and Majumbar imply that in the case of a growing number of particles N and in the case of larger dimensionality of the subsystems, i.e. growing number of degrees of freedom, the ratio of violation of the corresponding Bell-type inequality respectively increases and persists. Thus in this case –which is sometimes called the macroscopic limit– the local realistic and the quantum mechanical formalism diverge and do not converge. Now, what does this fact imply?

According to Zukowski this shows some fundamental discrepancy between the classical and quantum mechanical formalisms: "N-particle Bell-inequalities show us that quantum mechanical predictions for some states violate the inequalities by an amount that grows exponentially with N. The increasing number of particles, in this case does not bring us closer to the classical realm, but rather makes the discrepancies between quantum and classical even more profound" [88].

And according to Home the above mentioned divergence, has implications for classical and macroscopic ideas. "It is thus indicated that quantum mechanics implies a" strong" violation of classical realism even in the macroscopic domain......All the foregoing investigations corroborate the view that classical properties do not automatically emerge for "large" quantum systems, whatever "large" may mean: collections of a large number of subsystems N and/or states with large quantum numbers such as large spin j.[8]"

Thus according to Zukowski and Home the local realistic and quantum mechanical divergence has implications in the macroscopic domain and as well for taking the macroscopic limit. Although much can be said about ideas of a macroscopic domain and taking the macroscopic limit, here I will only discuss the following objection that the whole issue about the macroscopic domain of quantum mechanics is irrelevant. This objection can be phrased as follows. Perhaps the systems for which one gets a local realistic and quantum mechanical divergence do not occur in nature? Perhaps that the highly entangled states that give rise to the growing violations–although permitted by the quantum mechanical formalism– are ruled out through some other mechanism (one could think of decoherence)?

However, I myself believe that this objection misses a crucial point. Because whatever may be the case, the fact to be remembered and not to be ignored is that quantum mechanical and the local realistic formalisms diverge and not converge for large particle number and large quantum number. This has to deal with comparing formalisms, what does or does not occur in nature is not at stake here.

5.2.2 Non-violations

In the previous section the conceptual issue was the *violation* of specific Bell-type inequalities for the different possible measurement configurations determined by the size and dimension of the total system.

However, what about *non-violations*? What states can not be made to violate Bell-type inequalities? As we have seen, all inequalities are violated by certain entangled states. But does the converse hold as well? Do all entangled states violate a Bell-type inequality, i.e. are there no entangled states that do not violate a Bell-type inequality? In order to answer these question I will now consider the known results [58] about non-violations.

Separable states

The set of fully separable states (i.e. completely non-entangled states) is known to have a local HV-model for all possible multi-particle systems and all measurement configurations that are possible on these systems. This is the reason that these states are also called 'classically correlated states'.

Let me recall the definition of these states. Suppose one has a N-particle system where each system i has dimension d_i, The fully separable states are then the states that can be written as a convex sum of full N-particle direct-product states:

$$\rho = \sum_i p_i \rho_i^{(1)} \otimes \rho_i^{(2)} \ldots \otimes \rho_i^N, \tag{5.19}$$

with $\sum_i p_i = 1$, and where each ρ_i is a one-particle density operator for each of the the subsystems. These states have the special property that measurements give expectation values for all observables that are convex sums of expectation values of observables that act on the single subsystems:

$$E^{QM}(\hat{A}^{(1)}, \ldots, \hat{A}^N) = \mathrm{Tr}[\rho \hat{A}^{(1)} \otimes \ldots \otimes \hat{A}^N] = \sum_i p_i \mathrm{Tr}[\rho_i^{(1)} \otimes \hat{A}^{(1)}] \ldots \mathrm{Tr}[\rho_i^N \otimes \hat{A}^N]. \tag{5.20}$$

Now why do these states have a local HV-model for all possible measurement configurations and why are they also called 'classically correlated states'? Let me try to explain. The latter is due to the fact that the preparation procedure for these states can be completely obtained using only classical elements in the following sense [65]. Suppose one has N different preparing devices each preparing a specific state ρ_j depending upon the input i. Next use a random generator – chosen a classical device– that produces the inputs i each with a probability p_i. Then using these devices one produces the fully separable states of Eq.(5.19). Note however that this does not mean that the states have to be actually prepared in this matter, but only that their properties can be reproduced using this classical mechanism.

Further, as stated above, these states all allow for the construction of a local HV-model for all possible expectation values that these states give rise to. Let me show this. The observables of subsystem 1 are self-adjoint operators with spectral resolution $\hat{A}^{(1)} = \sum_\mu a_\mu^{(1)} P_\mu^{(1)}$, i.e. eigenvalues $a_\mu^{(1)}$ and eigenprojections P_μ, and similarly for all other subsystems.

Then the state $\rho \in \mathcal{H}^{(1)} \otimes \ldots \otimes \mathcal{H}^{(N)}$ admits a local hidden variable model if there is a hidden variable space Λ, a probability distribution $M(\lambda)$ and response functions $A^{(1)}(\mu, \lambda_i) \ldots A^N(\nu, \lambda_i)$ for all subsystem observables such that for all $\hat{A}^{(1)}, \ldots, \hat{A}^N$ and for all eigenvalues of all projection operators $P_0 i$,

$$\int d\lambda M(\lambda) A^{(1)}(\mu, \lambda) \ldots A^N(\nu, \lambda) = \mathrm{Tr}[\rho P_\mu^{(1)} \otimes \ldots \otimes P_\nu^N] \tag{5.21}$$

The claim now is that all classically correlated states, i.e. the fully separable states of Eq. (5.19) obey the condition of Eq.(5.21) and thus admit local HV-models. Hence they will satisfy all Bell inequalities for every measurement configuration (N, m, d). This can be proven by taking $\Lambda = \{1, \ldots, N\}$, $M(\lambda_i) = p_i$ and response functions $A^{(1)}(\mu, \lambda_i) = \mathrm{Tr}[\rho_i^{(1)} P_\mu^{(1)}]$ and similarly for the other observables. Then Eq.(5.20) implies Eq.(5.21). The observables are unrestricted and can thus have finite number of m different outcomes. Further, since each inequality for a measurement configuration consists of a sum of expectation values such as given in Eq.(5.21) all such inequalities for all possible measurement configurations and for the fully separable states of any N-particle system, where each subsystem can have any dimension, can be locally realistically modeled and thus these inequalities will not be violated. Thus this proves that any fully separable state allows for the construction of a hidden variable model for all possible measurement configurations (N, m, d). Note that the above only holds for full factorisability and ordinary local HV-theories. The extension to partial factorisability and partial local HV-theories will be performed in later sections.

To put the result of this subsection into perspective, let me present the logical result:

- non-entangled (i.e. separable) states $\Longrightarrow$ the existence of local HV-model.

Having this is mind one could ask if the converse is true as well. I.e. is every state admitting a local HV-model non-entangled? For pure bi-particle states and the measurement configuration $(2, 2, 2)$ we have seen in section 5.2.1 that indeed the converse is true: Every state admitting a local HV-model must be separable. However, for more general mixed states Werner has shown in 1989 the remarkable result that this is not true by explicit construction of a local HV-model for a family of entangled quantum states. In the next subsubsection this family of states is presented.

Werner states

A specific set of states derived by Werner [65], now also called the *Werner states*, has the property that despite being entangled a local HV-theory exists for these states for the measurement configuration $(2, M, d)$. Hence they do not violate Bell-type inequalities for these configurations. Werner was able to show two difficult things: (i) that these states are non-entangled and (ii) that a local HV-model exists for all possible experiments in the measurement configuration $(2, M, d)$. The trick he used was to make extensive use of symmetry.

Werner considered only states on the Hilbert spaces $\mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$ with $\mathcal{H}^{(1)} \cong \mathcal{H}^{(2)} \cong \mathbb{C}^d$ where each system has equal dimension d. He considered states that are given by density operators ρ satisfying $\rho = (\hat{U} \otimes \hat{U})\rho(\hat{U}^* \otimes \hat{U}^*)$. These mixed states are also called $U \otimes U$ invariant states and have the form:

$$\rho_W = \frac{1}{d^3}\mathbb{1} \otimes \mathbb{1} + \frac{2}{d^2}P^{anti} = \frac{1}{d^3}\mathbb{1} \otimes \mathbb{1} + \frac{1}{d^2}\sum_{i<j;i,j=1}^{d} |\,\phi_{i,j}\rangle\,\langle\,\phi_{i,j}|\,, \tag{5.22}$$

where P^{anti} is the projection onto the completely anti-symmetric subspace of $\mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$ and $|\,\phi_{i,j}\rangle$ is the 'spin-1/2 singlet state'

$$|\,\phi_{i,j}\rangle = \frac{1}{\sqrt{2}}(|\,i\rangle_1\,|\,j\rangle_2 - |\,j\rangle_1\,|\,i\rangle_2), \tag{5.23}$$

where $\{|\,i\rangle_1\}$, $\{|\,i\rangle_1\}$ are orthonormal bases in $\mathcal{H}^{(1)}, \mathcal{H}^{(2)}$ respectively. The important property of these mixed states is that they are not separable, i.e. they are entangled. Furthermore, Werner has proven that these states allow for the construction of a local HV-model for all possible expectation values of orthodox measurements that they give rise to. Let me show this construction.

The observables of subsystem 1 are self-adjoint operators with spectral resolution $\hat{A}^{(1)} = \sum_\mu a_\mu^{(1)} P_\mu^{(1)}$, i.e. eigenvalues $a_\mu^{(1)}$ and eigenprojections $P_\mu^{(1)}$ with $\sum_\mu P_\mu^{(1)} = \mathbb{1}$, and similarly for the other subsystem: $\hat{A}^{(2)} = \sum_\nu a_\nu^{(2)} P_\nu^{(2)}$, $\sum_\nu P_\nu^{(2)} = \mathbb{1}$. Then the state $\rho \in \mathcal{H}^1 \otimes \mathcal{H}^2$ admits a local hidden variable model if there is a hidden variable space Λ, a probability distribution $M(\lambda)$ and response functions $A^{(1)}(\mu, \lambda), A^{(2)}(\nu, \lambda)$ for all subsystem observables such that for all $\hat{A}^{(1)}, \hat{A}^{(2)}$ and for all eigenvalues of all projection operators P_i,

$$\int d\lambda M(\lambda) A^{(1)}(\mu, \lambda) A^{(2)}(\nu, \lambda) = \mathrm{Tr}[\rho P_\mu^{(1)} \otimes P_\nu^{(2)}]. \tag{5.24}$$

The claim now is that all classically correlated states, i.e. the fully separable states of Eq. (5.19), fulfill Eq.(5.24) and thus admit local HV-models and hence satisfy all Bell inequalities for every measurement configuration (N, m, d). This can be proven as follows. Take Λ the unit sphere $\{\lambda \in \mathbb{C}^d | \, |\lambda| = 1\}$ and the choice

$$\begin{aligned} A^{(1)}(\mu, \lambda) &= \langle \lambda | P_\mu^{(1)} \lambda \rangle, \\ A^{(2)}(\nu, \lambda) &= \begin{cases} 1, & \langle \lambda | P_\nu^{(1)} \lambda \rangle < \langle \lambda | P_\mu^{(1)} \lambda \rangle \ \forall \mu \neq \nu, \\ 0, & \text{else}, \end{cases} \end{aligned} \tag{5.25}$$

then it can be shown [65, 58] that Eq. (5.24) holds.

Thus specific states exist for which, despite being entangled, a local HV-theory exists for these states for the measurement configuration $(2, M, d)$ and thus they do not violate Bell-type inequalities for these configurations. This implies that entanglement is not sufficient for the non-existence of a local HV-model. The logical form of this result is as follows:

- Existence of LHV model $\not\Rightarrow$ Separable state.

Hidden Entanglement.

This last logical result shows us the following consequence:

> The requirement of having a separable quantum description of two subsystems is a much more stringent condition than the requirement of admitting a factorisable description, i.e. admitting any possible local HV-model.

This feature allows for hidden entanglement,i.e entanglement that cannot be revealed using orthodox local measurements testing a Bell-type inequality.

The previous is only valid for the case of orthodox quantum measurements because the HV-theories treated so far are only required to model projective measurements, i.e. they have to obey the quantum criterium for the orthodox quantum formalism.

However, for general measurements using the generalized quantum formalism this logical result does not hold. Although it is the case that the Werner states, despite being entangled, cannot violate any Bell inequality for usual projective measurement, nevertheless, as shown by Popescu [52], they show violation if subjected to generalized measurement that use POVMs (for example a sequence of local measurements or some local distillation operations). This feature is called 'revealing hidden entanglement' [52]. Thus the following question remains unanswered: Is entanglement sufficient or not for the non-existence of a local HV-model when this local HV-model is subjected to the requirement of reproducing all quantum mechanical predictions not only for orthodox but also for general measurements? In other words, can all hidden entanglement be revealed? This question will be extensively treated in chapter 6 when the generalization of orthodox to general quantum measurements will formally take place.

PPT-states

Another set of states that cannot be made to violate a specific, though rather general set of Bell inequalities is the set of positive partial transpose states, the so-called PPT-states.

We have already seen in section 3.3.1 that the PPT criterium is a necessary criterium for separability and a sufficient one for non-distillability: all separable states are PPT-states and all PPT-states are non-distillable. However positivity of any partial transposition is also sufficient for non-violation of any generalized Mermin (i.e Bell-Klyshko) inequality $E^{\text{lr}}(F_N) \leq 2$ of Eq.(4.74) for the measurement configuration $(N, 2, 2)$. Werner and Wolf [26] obtained this result by showing that $|E_\rho(\hat{F}_N)| = \text{Tr}[\rho \hat{F}_N] \leq 2$ for any ρ that has positive partial transposition with respect to all partitions of the multi-particle state in to two subsystems, i.e for any ρ that is a PPT-state. Here $\hat{F}_N$ is the N-particle Bell-operator for the measurement configuration $(N, 2, 2)$ defined in Eq.(4.75). The proof of this result is rather extensive and is here omitted. The logical result is:

- PPT-states $\Longrightarrow$ non-violation of Bell inequality for $(N, 2, 2)$.

In order to use this result in an interesting way, I will have to recall from section 3.1.2 that although the PPT-criterium is sufficient for separability, it not necessary. Indeed, there are entangled states that have positive partial transposition [64]. Now using the above result that all PPT-states do not violate a Bell inequality for $(N, 2, 2)$, these entangled states consequently do not violate such a Bell inequality and thereby thus admit a local-HV model. Furthermore because all PPT-states are undistillable these states are referred to as PPT *bound* entangled states. The existence of such bound entangled states admitting a local-HV model was first shown by Horodecki [64].

However, do all bound entangled states admit a local HV-model? Dür [67] proved that this is not the case by constructing multi-particle bound entangled states that do not admit a LHV model because they violate a specific Bell-inequality. The implications of this result are that violation of a Bell-type inequality is not sufficient for distillability and further that some bound entangled states violate local realism[67].

The construction by Dür of these multi-particle states is as follows. For a certain set of mixed states ρ_N–which are here not specified– he shows that the states are bound entangled (non-separable and non-distillable) for $N \geq 8$ and furthermore that they violate the Bell-Klyshko inequality for $N \geq 8$. Thus for N greater or equal to eight there exist bound entangled states violating local realism.

Open Questions

There remain a number of open problems concerning the relation of (in-)separability to the existence of a local HV-model. Here I mention two.

1. It is not known whether or not all bound entangled states for $N < 8$ can be described by a local HV-theory [67].
2. What mathematical property of density matrices leads to sufficient and *necessary* conditions for compatibility with local-HV theories? Peres [78] conjectures that positive partial transposition (PPT) is sufficient and necessary. In general both are as as yet unproven, although as shown above it is the case that all PPT states will obey a Bell-inequality for $(N, 2, 2)$. However, without further requirements, the necessity cannot be since the Werner states are *not* PPT and nevertheless cannot violate a Bell-inequality. Perhaps that with the extra assumption of distillability the necessity could be shown since the Werner states can be distilled so as to end up violating a Bell-inequality. This is the earlier discussed feature of revealing hidden entanglement.

5.3 Local HV-theory Formalism vs. Quantum Mechanical State Space

All the results of the previous sections and chapters about the relation between the quantum state space structure and the local HV-theory formalism will be here summarized and put together in figures.

- Local HV-model $\not\Longrightarrow$ Separable state. Section 5.2.2.
- PPT-states $\Longrightarrow$ Non-violation Bell inequality for $(N, 2, 2)$. Section 5.2.2.
- Non-entangled (i.e. separable) states $\Longrightarrow$ local HV-model. Section 5.2.2.
- Local HV-model $\Longrightarrow$ non-violation of Bell inequality. Section 4.2.4.
- Non-violation of complete set of Bell inequality for (N,2,2) $\Longrightarrow$ local HV-model. Section 4.4.1.
- Conjecture by Peres: PPT $\Longleftrightarrow$ local HV-model. Section 5.2.2.
- Non-violation of Bell inequality $\Longrightarrow$ non-distillability. Section 5.2.2.
- Non-distillability $\not\Longrightarrow$ non-violation of Bell inequality. Section 5.2.2.

- Separability $\Longrightarrow$ PPT. Section 3.1.2.
- PPT $\not\Longrightarrow$ Separability. Section 3.1.2.
- PPT $\Longrightarrow$ non-distillability. Section 3.3.1.
- Non-distillability $\not\Longrightarrow$ PPT. Section 3.3.1.

All these results will be put in the following two diagrams. They were inspired by Werner *et al.* [58], but greatly modified.

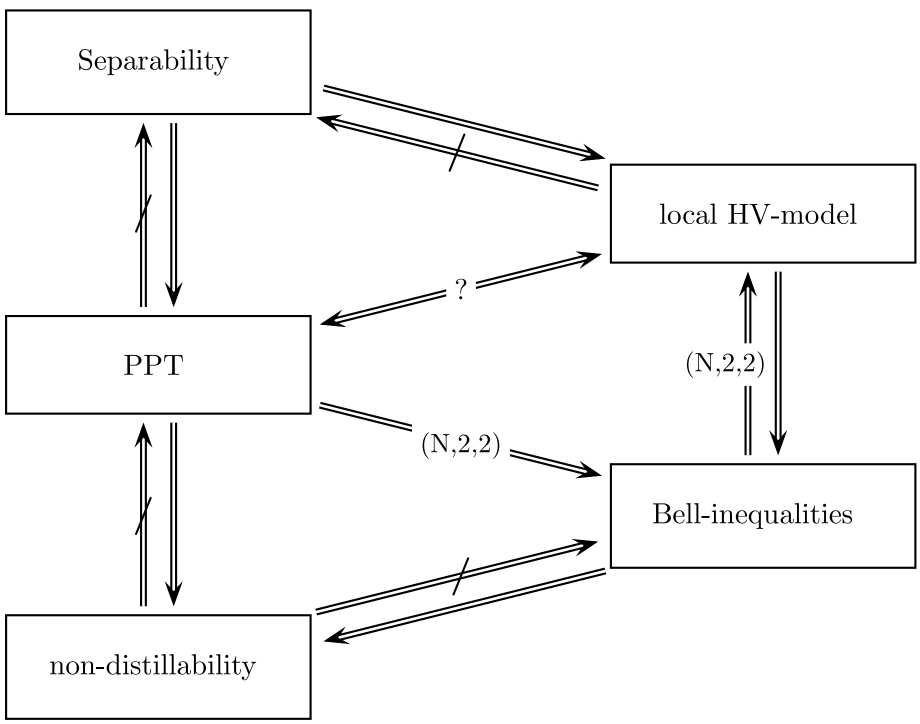


Figure 5.2: Separability structure (left) related to hidden variable structure (right) for general quantum states. The question marks '?' indicate the as yet unproven conjecture of Peres.

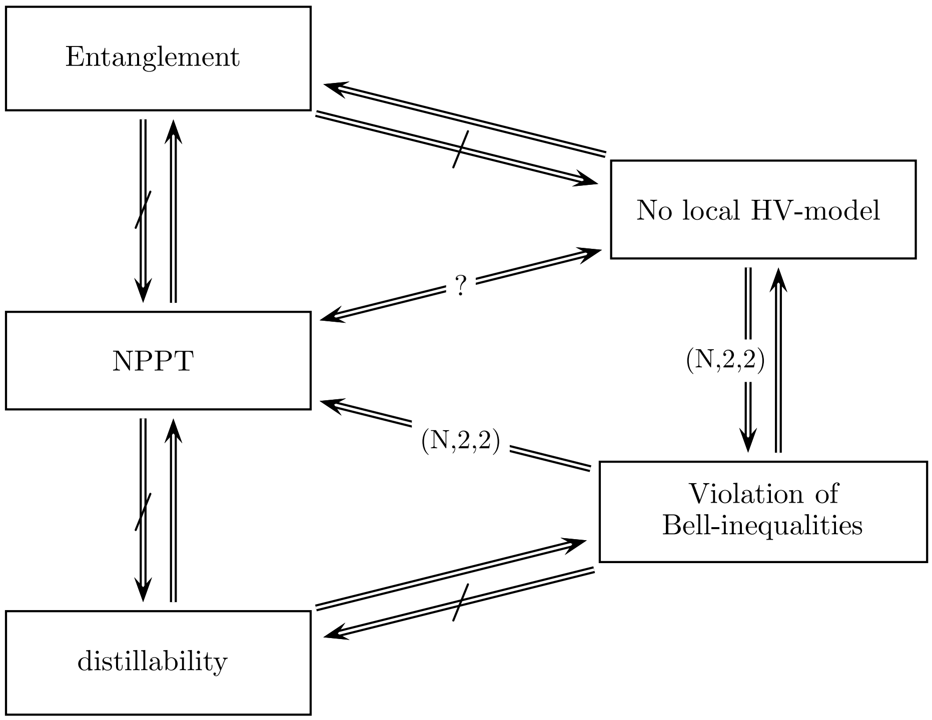


Figure 5.3: Negation of figure 5.2. Entanglement structure (left) related to hidden variable structure (right) for general quantum states. The question marks '?' indicate the as yet unproven conjecture of Peres.

5.4 Extension to Partial Factorisability: Quantum Mechanical (Non-)Violations of the Svetlichny-inequalities.

All the cases of (non-)violations of Bell-type inequalities that have been treated in this chapter use inequalities that address *full* separability of all particles. The case of (non)-violations Bell-type inequalities for *partial* factorisability has not yet been treated. This will be the topic of this subsection.

However, no full investigation will be performed of all possible systems (i.e. variation of both number of particles N and $dim\mathcal{H}$ of the Hilbert spaces) and measurement configurations (N, m, d) as was done for full factorisability. Only dimension $\mathcal{H} = 2$ per particle and measurement configurations $(N, 2, 2)$ will be considered. Thus no other inequalities are considered than the N- particle Svetlichny inequalities of section 4.4.2. The known results about quantum mechanical violations and non-violations of these

Further, given the recent experimental interest in quantum correlations in 3- and 4-particle systems and the probable extension to even larger number of particles, it becomes relevant to determine whether such correlations are due to full N-particle quantum entanglement and not just classical combinations of quantum entanglement of a smaller number of particles. I show the Svetlichny inequalities addresses this question and provide explicit means to answer it.

This investigation has a remarkable result which treated in the next subsection. The feature of hidden entanglement again shows up. For it is the case that analogous to the bi-particle case where certain states (the Werner states) despite being entangled nevertheless could not be made to violate a Bell inequality, certain N-particle states, despite being fully entangled, can not be made to violate a Svetlichny inequality. However there is one important difference. In the bi-particle case the states not violating any Bell inequality were explicitly shown to have a local HV model whereas it is unknown whether or not the fully entangled N-particle states not violating any Svetlichny inequality allow for a partial local HV model. Nevertheless the question whether or not the full N particle entanglement of these states can be revealed becomes relevant and motivates the study of this form of hidden entanglement.

To set the terminology, recall that the Svetlichny inequalities of Eq.(4.91) can be expressed as:

$$|\sum_{I^\pm} \sigma(I^\pm) E(A_{i_1}^{(1)} \cdots A_{i_N}^{(N)})| = |\langle S_N^\pm \rangle| \leq 2^{N-1}. \tag{5.26}$$

With $I^\pm = (i_1, i_2, \ldots, i_N)$ the specific sequences that generate the two Svetlichny inequalities and $\sigma_I^\pm = \pm 1$ is a sign for each N-tuple I. And further recall that the fidelity criterium

$$F(\rho) := \langle \psi_{\text{GHZ}}^N | \rho | \psi_{\text{GHZ}}^N \rangle \geq 1/2 \ ,$$

is a sufficient criterium for the N-particle state ρ to be N-particle entangled, where $|\psi_{\text{GHZ}}^N\rangle$ is the N-particle GHZ state: $\frac{1}{\sqrt{2}}(|\uparrow\uparrow \cdots \uparrow\rangle + |\downarrow\downarrow \cdots \downarrow\rangle)$.

5.4.1 Quantum Mechanical Violations.

No systematic study of states violating the Svetlichny inequalities was performed. Here I present my own results.

(i) The pure N-particle GHZ states $\left|\psi_{\text{GHZ}}^N\right\rangle$ provide the maximal violation of any Svetlichny inequality. See section 4.4.2 for proof.

(ii) The following family of mixed states gives a violation:

$$\rho_S^N = \alpha \left|\psi_{\text{GHZ}}^N\right\rangle \left\langle \psi_{\text{GHZ}}^N\right| + \frac{\beta}{2^N}\mathbb{1} \ , \tag{5.27}$$

with $\alpha + \beta = 1$ and $\frac{1}{\sqrt{2}} < \alpha \leq 1$.

This set gives a fidelity $F \geq 1/2$ and is thus full N-particle entangled and will violate any of the Svetlichny inequalities, i.e. $S' > 2^{N-1}$ with S' the largest value for all possible Svetlichny inequalities for all measurement configurations $(N, 2, 2)$ applicable to these states. For proof see 5.4.2.

5.4.2 Non-violations.

Just as in the previous case of states that give violations, again no systematic study was performed about the states non-violating the Svetlichny inequalities. However a certain set of states, here treated last, was examined rather thoroughly since it gives rise to questions about hidden entanglement.

(i) All non-fully entangled states can not be made to violate a Svetlichny inequality. Thus all M-particle entangled N-particle systems with $M < N$, $M = 1, 2 \ldots N-1$, (i.e. including all partially and all fully separable states).

The proof is simple: Because violation of Svetlichny inequalities is sufficient for full N-particle entanglement – as proven in section 4.4.2–, the negation of this implies that the non-fully entangled states cannot violate the Svetlichny inequalities.

(ii) Some fully N-particle entangled states can not be made to violate a Svetlichny inequality. Not the pure but mixed ones. This is possible since violation of Svetlichny is only sufficient for full entanglement and not necessary. I have investigated only a small set of such states.

Consider the family of mixed states of Eq. (5.27) with $\frac{1}{2} < \alpha < \frac{1}{\sqrt{2}}$.

This set gives a fidelity $F \geq 1/2$ and is thus full N-particle entangled. However there is no violation since $S' \leq 2^{N-1}$ with S' the largest value for all possible Svetlichny inequalities for all measurement configurations $(N, 2, 2)$ applicable to these states. For proof see next subsection. The implication of this result is that the impossibility to violate the Svetlichny inequalities does not imply some form of partial separability. We get a situation analogous to the existence of the bi-partite Werner states which show that the impossibility to violate the CHSH inequality does not imply that the states are separable. In order to show this analogy the Werner states will again be treated but now using a different formulation. In the following subsubsection I will use the same formalism to treat the case of $N = 3$ and the case of general N.

Full N-particle Entangled States not Violating the Svetlichny-inequalities.

In this subsubsection I will show the existence of full N-particle entangled states that do not violate a Svetlichny inequality for the case of $N = 2$, $N = 3$ and for general N.

▶ Two-particle, $N = 2$.

Look at the bi-particle GHZ state: $|\,\psi^2_{GHZ}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$. Use the fidelity-criterium: $F = \langle\,\psi^2_{GHZ}|\,\rho\,|\,\psi^2_{GHZ}\rangle \geq 1/2 \implies \rho$ is entangled. Further, look at the operators $A \otimes B$, $A \otimes B'$, $A' \otimes B$, $A' \otimes B'$ which are used in the CHSH-inequality.

Choose as A, B etc. spin-operators of the form:

$$\begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix}$$

And choose a set of directions and angles such that we get a maximal violation of the CHSH- inequality One such set is:

$$\vec{a} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \vec{a'} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \vec{b} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \vec{b'} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

with all vectors in the x, y-plane.

Then, the sum $A'B' + AB' + B'A - AB$ is equal to :

$$2\sqrt{2}\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

This result has a remarkable feature. Look at the bi-particle GHZ state $|\,\psi^2_{GHZ}\rangle$. It has density matrix:

$$\frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

and the other GHZ state $|\,\phi^2_{GHZ}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)$ is

$$\frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}$$

Then the following holds:

$$\frac{A'B' + AB' + B'A - AB}{2\sqrt{2}} = \left|\,\psi^2_{GHZ}\right\rangle\left\langle\,\psi^2_{GHZ}\right| - \left|\,\phi^2_{GHZ}\right\rangle\left\langle\,\phi^2_{GHZ}\right|. \tag{5.28}$$

That is, the sum of local operators is also the sum of two entangled (density) operators. In terms of expectation values, for all ρ the following holds:

$$\begin{aligned} &\mathrm{Tr}[\rho\frac{A'B' + AB' + B'A - AB}{2\sqrt{2}}] = \\ &\mathrm{Tr}[\rho\left|\,\psi^2_{GHZ}\right\rangle\left\langle\,\psi^2_{GHZ}\right|] - \mathrm{Tr}[\rho\left|\,\phi^2_{GHZ}\right\rangle\left\langle\,\phi^2_{GHZ}\right|] \leq \mathrm{Tr}[\rho\left|\,\psi^2_{GHZ}\right\rangle\left\langle\,\psi^2_{GHZ}\right|] \end{aligned} \tag{5.29}$$

Violation of the CHSH inequality implies that the left part of Eq.(5.29) is greater than or equal to $1/\sqrt{2}$. Density matrices (i.e. states) that provide such a violation then must have a fidelity measure $F \geq 1/\sqrt{2}$. In logical form:

- CHSH $\geq 2 \Longrightarrow F \geq 1/\sqrt{2}$. (5.30)

I conjecture that for all ρ and all CHSH inequalities a measure F exists such that the above holds. Thus I conjecture that violation of CHSH implies violation of fidelity-criterium but not necessarily the other way around.

–Example:

Consider the Werner states.

$$\rho_W = \frac{1}{8}\mathbb{1} \otimes \mathbb{1} + \frac{1}{2}\left|\,\psi^2_{GHZ}\right\rangle\left\langle\,\psi^2_{GHZ}\right|. \tag{5.31}$$

1) These states are not separable, i.e. they are entangled! This follows because the fidelity F is equal to $1/2$, just enough for the state to be entangled.

2) As was treated in section 5.2.2, a local HV-model exists for all orthodox measurements performed on these states and thus no Bell-inequality will be violated using this state.

This example allows for the following implication: Specific quantum states exist that are truly two-particle entangled (they have a fidelity above 1/2) but they can not be made to violate the CHSH-inequality. They are said to be hidden entangled.

▶ Three-particle Case, $N = 3$.

Take the Svetlichny-inequality

$$\begin{aligned} &| \, E(ABC) + E(ABC') + E(A'BC) + E(AB'C) - E(A'BC') \\ &\quad -E(AB'C') - E(A'B'C) - E(A'B'C') \, | \leq 4, \end{aligned} \tag{5.32}$$

with $E(ABC) = \mathrm{Tr}[\rho A \otimes B \otimes C]$ and A, B, C the spin operators

$$\begin{pmatrix} n_z & n_x - i n_y \\ n_x + i n_y & -n_z \end{pmatrix}.$$

Consider the state: $|\,\psi^3_{\mathrm{GHZ}}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\rangle)$. For this state $E_{QM}(a,b,c) = \langle \mathbf{a}\sigma \otimes \mathbf{b}\sigma \otimes \mathbf{c}\sigma \rangle = \cos(\alpha + \beta + \gamma)$, with $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ unit-vectors in the xy-plane with angles α, β and γ with respect to the x-axis. For $\alpha = 0$, $\alpha' = -\pi/2$, $\beta = \pi/4$, $\beta' = -\pi/4$, $\gamma = 0$ and $\gamma' = -\pi/2$ the inequality (5.32) is violated maximally with the value $4\sqrt{2}$.

The sum $ABC + ABC' + A'BC + AB'C - A'BC' - AB'C' - A'B'C - A'B'C'$ is equal to

$$4\sqrt{2} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

The GHZ-state $|\,\psi^3_{\mathrm{GHZ}}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\rangle)$ has the following density matrix:

$$\frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

And the state $|\,\phi^3_{\mathrm{GHZ}}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\rangle - |\downarrow\downarrow\downarrow\rangle)$ has the almost identical density matrix:

$$\frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

It then follows that:

$$\frac{ABC + ABC' + A'BC + AB'C - A'BC' - AB'C' - A'B'C - A'B'C'}{4\sqrt{2}} = \left|\,\psi^3_{\mathrm{GHZ}}\right\rangle\left\langle\,\psi^3_{\mathrm{GHZ}}\right| - \left|\,\phi^3_{\mathrm{GHZ}}\right\rangle\left|\,\phi^3_{\mathrm{GHZ}}\right\rangle. \quad (5.33)$$

So again it follows that the sum of local operators is also the sum of two entangled (density) operators! Next, we get the result for the sum of the expectation values:

$$\mathrm{Tr}[\rho\frac{ABC + ABC' + A'BC + AB'C - A'BC' - AB'C' - A'B'C - A'B'C'}{4\sqrt{2}}] = \mathrm{Tr}[\rho\left|\,\psi^3_{\mathrm{GHZ}}\right\rangle\left\langle\,\psi^3_{\mathrm{GHZ}}\right|] - \mathrm{Tr}[\rho\left|\,\phi^3_{\mathrm{GHZ}}\right\rangle\left|\,\phi^3_{\mathrm{GHZ}}\right\rangle] \leq \mathrm{Tr}[\rho\left|\,\psi^3_{\mathrm{GHZ}}\right\rangle\left\langle\,\psi^3_{\mathrm{GHZ}}\right|]. \quad (5.34)$$

Violation of the Svetlichny inequality implies that the left part of Eq.(5.34) is greater than or equal to $1/\sqrt{2}$. Density matrices (i.e. states) that provide such a violation then must have a fidelity measure $F \geq 1/\sqrt{2}$. I conjecture that for all ρ and all Svetlichny inequalities a measure F exists such that the above holds Thus I conjecture that violation of Svetlichny-inequality implies violation of fidelity measure $F \leq 1/2$, but not necessarily the other way around. In logical form:

- Svetlichny inequality $\geq 4 \Longrightarrow F \geq 1/\sqrt{2}$. (5.35)

–Example:
We are searching for fully three-particle entangled states that do not violate the Svetlichny-inequality. These states must have the following properties. First they must have a fidelity F greater than $\frac{1}{2}$. Second, the states cannot be made to violate any three-particle Svetlichny inequality S for all possible local measurements.

Now consider the following family of states:

$$\rho_S^3 = a \left| \psi_{\mathrm{GHZ}}^3 \right\rangle \left\langle \psi_{\mathrm{GHZ}}^3 \right| + b\frac{\mathbb{1}}{8}, \tag{5.36}$$

with $a+b=1$ and $\frac{3}{7} \leq a \leq \frac{1}{\sqrt{2}}$. ($\mathbb{1}$ is the identity-operator). I will now proof the following two statements

1) $\forall \rho_S^3: \quad F \geq \frac{1}{2}$ for all allowable a. Thus these states are entangled.

2) $\forall \rho_S^3: \quad \mathrm{Tr}[\rho S] \leq 4$ for all a, for all three-particle inequalities S and for all possible sets of local measurements. Thus these states can not violate any of the Svetlichny inequalities.

The proof of these statements is as follows. First, the mixture ρ has a fidelity of $\langle \psi_t | \rho \; | \psi_t \rangle = a + b/8$. Using the fact that $a+b=1$ and $\frac{3}{7} \leq a \leq \frac{1}{\sqrt{2}}$, it follows that $F \geq \frac{1}{2}$.
Next, note that $Tr[\frac{\mathbb{1}}{8}S] = 0$ for all possible spin-measurements and all possible S. This can be easily seen by considering the product of any three arbitrary spin observables (in the arbitrary directions $\mathbf{a}, \mathbf{b}$ and $\mathbf{c}$) and noting that $E_{QM}(A,B,C) = \langle \mathbf{a}\sigma \otimes \mathbf{b}\sigma \otimes \mathbf{c}\sigma \rangle = 0$ for the completely random state $\rho = \frac{\mathbb{1}}{8}$.

Furthermore $\mathrm{Tr}[| \psi_{\mathrm{GHZ}}^3 \rangle \langle \psi_{\mathrm{GHZ}}^3 | S]$ has a maximal value of $4\sqrt{2}$ for all possible S and some specific set of observables. (See for example the previous section for such a set of observables for a certain S).Now suppose we take a certain S and such a set of observables that indeed $\mathrm{Tr}[| \psi_{\mathrm{GHZ}}^3 \rangle \langle \psi_{\mathrm{GHZ}}^3 | S] = 4\sqrt{2}$. For any different S or any different set of observables this is never greater than $4\sqrt{2}$.

This fact implies that $\mathrm{Tr}[\rho S] \leq 4\sqrt{2}\, a + 0$ and thus $\mathrm{Tr}[\rho S] \leq 4$ for all allowable a (with ρ given in Eq.(5.36). This holds for all possible S and all possible sets of observables.

–Conclusion: The family of states in Eq.(5.36) is truly three-particle entangled, but cannot be made to violate any Svetlichny inequality S for all possible sets of orthodox observables. The entanglement in these states cannot be revealed using a Svetlichny inequality (or any other N-particles inequality) and I therefore call these states hidden entangled.

▶ Multi-particle Case, N arbitrary.

Consider the $2^N \times 2^N$ density matrix of the N-particles GHZ state: $\left| \psi_{\mathrm{GHZ}}^N \right\rangle \left\langle \psi_{\mathrm{GHZ}}^N \right|$. This $N \times N$ density matrix in the z-basis has only four elements, all equal to $1/2$, on the far diagonal and far off-diagonal positions (Positions $(1,1),(N,N)$ and $(1,N),(N,1)$ respectively.) Now we focus at the case where this state gives a maximal violation of the above used Svetlichny inequality. That is, we have $\mathrm{Tr}[S' \,|\, \psi^N_{\mathrm{GHZ}} \rangle \langle \psi^N_{\mathrm{GHZ}} |] = 2^{N-1}\sqrt{2}$. With S' the specific S which allows such a maximal violation. (Note that any other S gives a smaller violation.) In order for this maximal violation to hold, we get that for the matrix representation of S' in the z-basis with elements a, b, c, d on positions $(1,1), (N,1), (1,N)$ and (N,N) respectively, the following must hold: $1/2(a+b+c+d) = 2^{N-1}\sqrt{2}$. Because the spin observables (i.e. Pauli-matrices) are in the xy-plane it follows that all diagonal elements of S' are zero. Furthermore from symmetry of the Pauli-matrices it follows that the far-off diagonal elements are equal. This gives the solutions for a, b, c, d: $a = d = 0$ and $b = c = 2^{N-1}\sqrt{2}$. Thus the matrix representation of S' has only two non-zero elements, i.e. the far-off diagonal elements equal to $2^{N-1}\sqrt{2}$, whereas the rest are all zero.

Upon explicitly considering the $2^N \times 2^N$ density matrices for the GHZ states $|\, \psi^N_{\mathrm{GHZ}} \rangle$ and $|\, \phi^N_{\mathrm{GHZ}} \rangle$ one can easily see that

$$\frac{Tr[\rho S']}{2^{N-1}\sqrt{2}} = Tr[\rho(|\, \psi^N_{\mathrm{GHZ}} \rangle \langle \psi^N_{\mathrm{GHZ}} | - |\, \phi^N_{\mathrm{GHZ}} \rangle \langle \phi^N_{\mathrm{GHZ}} |)]. \tag{5.37}$$

In other words, the operator S', a sum of 2^N local observables, is equal to the sum of two entangled (density) operators.

We use this result to provide a link with the fidelity measure $F = Tr[\rho \,|\, \psi^N_{\mathrm{GHZ}} \rangle \langle \psi^N_{\mathrm{GHZ}} |]$ of the pure state $\rho \,|\, \psi^N_{\mathrm{GHZ}} \rangle$. We start with the following result:

$$\begin{aligned}\frac{Tr[\rho S']}{2^{N-1}\sqrt{2}} &= Tr[\rho(|\, \psi^N_{\mathrm{GHZ}} \rangle \langle \psi^N_{\mathrm{GHZ}} | - |\, \phi^N_{\mathrm{GHZ}} \rangle \langle \phi^N_{\mathrm{GHZ}} |)] \\ &\leq Tr[\rho \,|\, \psi^N_{\mathrm{GHZ}} \rangle \langle \psi^N_{\mathrm{GHZ}} |] = F,\end{aligned} \tag{5.38}$$

where ρ could be an arbitrary density matrix, S' is the above used Svetlichny operator and F is the fidelity measure of the state $|\, \psi^N_{\mathrm{GHZ}} \rangle$.

Violation of the N-particle Svetlichny inequality of Eq. (5.26) with $S^{\pm} = S'$ implies that the left part of Eq.(5.38) is greater than or equal to $1/\sqrt{2}$. Density matrices (i.e. states) that provide such a violation then must have a fidelity measure $F \geq 1/\sqrt{2}$. I conjecture that for all ρ and all inequalities S' a measure F exists such that the above holds. In other words, I conjecture that states violating the N- particle Svetlichny inequalities must have a fidelity $F \geq 1/\sqrt{2}$. In logical form:

- Svetlichny inequality $S' \geq 2^{N-1} \Longrightarrow F \geq 1/\sqrt{2}$. (5.39)

–Example:
Consider the set of states ρ^N_S

$$\rho^N_S = a \,|\, \psi^N_{\mathrm{GHZ}} \rangle \langle \psi^N_{\mathrm{GHZ}} | + \frac{b}{2^N}\mathbb{1} \tag{5.40}$$

with $\frac{1}{2} < a < \frac{1}{\sqrt{2}}$, $a + b = 1$ For this set of states the following two statements hold (The proof is analogous to the three particle case.):

1) $\forall \rho^N_S :\quad F \geq \frac{1}{2}$ for all allowable a. Thus these states are entangled.

2) $\forall \rho_S^N$: $\mathrm{Tr}[\rho S] \leq 2^{N-1}$ for all a, for all the N-particle inequalities S and for all possible sets of local measurements. Thus these states can not violate any of the Svetlichny inequalities.

–Conclusion: This example implies the following implication: Specific quantum states exist that are truly N-particle entangled ($F \geq 1/2$) but which can not be made to violate the Svetlichny inequality using orthodox measurements. This result using Eq.(5.39) holds for those states that have the largest violation of any possible Svetlichny inequality for the inequality with $S = S'$. The entanglement in these states cannot be revealed using a Svetlichny inequality (or any other N-particles inequality) and I therefore call these states hidden entangled.

A different way of expressing this is the following:

- Non-violation of Svetlichny inequalities $\not\Longrightarrow$ some form of partial separability.

Although the Svetlichny inequalities are only necessary tests for the existence of partial factorisability, they are not trivial ones. Further, because complete sets of Bell inequalities exist for full factorisability it could well be the case that such complete sets also exist for partial factorisability[2]. In that case these sets would provide necessary and sufficient conditions for partial factorisability to hold. I believe such a set to exist and therefore conjecture the following:

- Conjecture: Complete set of Svetlichny inequalities $\Longrightarrow$ existence of partial local HV-theory.

5.4.3 Partial Separability vs. Partial Factorisability.

We have seen the existence of the states ρ_S^N that are fully entangled N-particles states that however cannot be made to violate any Svetlichny inequality. This is analogous to the full factorisability case where some quantum states will not violate any Bell-type inequalities although being entangled. This was shown in the bi-partite case for the Werner states.

If my conjecture that a complete set of Svetlichny inequalities exists is true and that all these inequalities cannot be violated by these truly N-particle entangled (i.e. completely non-separable) states ρ_S^N then they would allow for a hidden variable model in which partial factorisability holds.

In other words, despite being truly entangled, it could be the case that these states nevertheless have a partial local HV-model. But perhaps there is some *hidden non-locality* [52] in these states that has to be revealed in other ways (e.g. using generalized measurements) to exclude the possibility of models in which partial factorisability holds.

All this can be viewed from a different perspective. Recall from the discussion of the Werner states that the requirement of having a separable quantum description of *two* subsystems is a much more stringent condition than the requirement of

[2] This problem is currently being worked on. George Svetlichny, private communication.

admitting a factorisable description, i.e. admitting any possible local HV-model. Analogously, I conjecture the following.

> The requirement of having a partially separable quantum description of the three or more subsystems is a more stringent condition than the requirement of admitting any possible partial local hidden variable model

Here I mean by a partially separable quantum description a description with a bi-separable or fully separable state, i.e. with e.g. $\rho_{AB} \otimes \rho_C$ or $\rho_A \otimes \rho_B \otimes \rho_C$. for a three-particle system $A+B+C$. Thus, if one would be able to find a necessary *and sufficient* set of Svetlichny inequalities for a partial local HV-model to exist, one would be able to proof the above mentioned conjecture.

5.5 Partial Local HV-models vs. the Quantum Mechanical State Space.

All the results of the previous sections and chapters about the relation between the quantum state space structure and the partial local HV-theory formalism will be here summarized and put together in figures.

- Partial local HV-theory $\Longrightarrow$ Non-violation of Svetlichny inequalities. Section 4.4.2.

- Partial/full separability $\Longrightarrow$ partial local HV-theory. Section 4.4.2.

- Partial/full separability $\Longrightarrow$ Non-violation of Svetlichny inequalities. Section 4.4.2.

- Non-violation of Svetlichny inequalities $\not\Longrightarrow$ partial separability. Section 5.4.3.

- Conjecture: Non-violation of Svetlichny inequalities $\Longrightarrow$ partial local HV-theory. Section 4.4.2.

- Conjecture: partial local HV-theory $\not\Longrightarrow$ partial separability. Section 5.4.3.

All these results will be put in figure 5.4 and in its negation in figure 5.5.

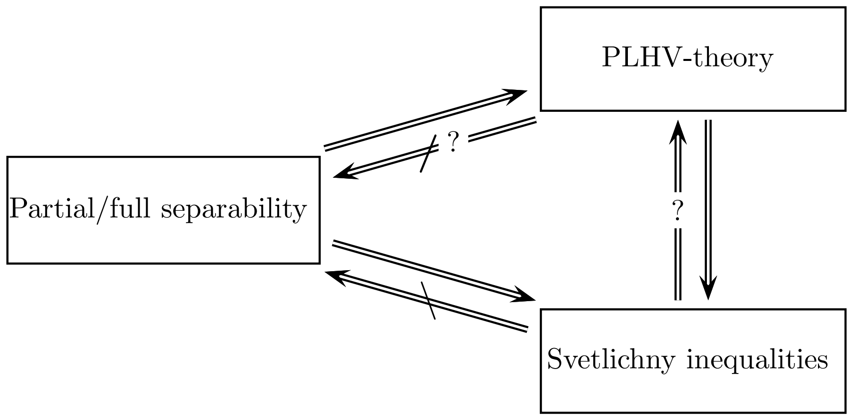


Figure 5.4: Entanglement structure (left) related to partial hidden variable structure (right) for general quantum states. The question marks '?' indicate the as yet unproven conjectures.

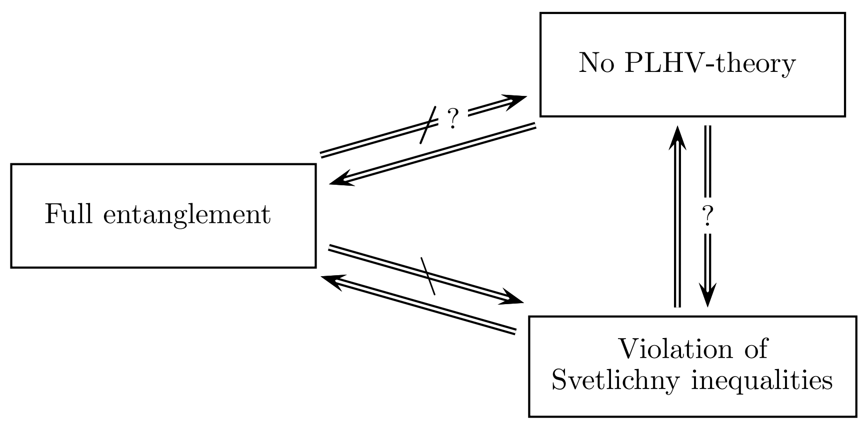


Figure 5.5: Negation of figure 5.4. Entanglement structure (left) related to partial hidden variable structure (right) for general quantum states. The question marks '?' indicate the as yet unproven conjectures.

5.6 Classification of Quantum States. Part IV.

- **Classically correlated states.** As presented in section 5.2.2 classically correlated states are the fully separable states, i.e convex sums of full N-particle direct-product states: These states have the special property that measurements give expectation values for all observables that are convex sums of expectation values of observables that act on the single subsystems and thus they have a local HV-model for all possible measurement configurations.

- **Werner states or $U \otimes U$ states.** Werner states are mixed bi-particle states that are entangled but nevertheless allow for a local HV model for all projective measurements. They are $U \otimes U$ symmetric states See section 5.2.2.
- **PPT bound entangled states.** These are PPT-states –and thus undistillable– that are entangled. See section 5.2.2.
- **Hidden entangled states.** These states are entangled but cannot be made to violate a Bell-type inequality (full factorisability) or Svetlichny inequality (partial factorisability) using orthodox measurements. Examples are the Werner states, the PPT bound entangled states, and the fully entangled set ρ_S^N of Eq.(5.40).

5.7 Conclusion and Summary

This chapter is largely devoted to quantum mechanical violations and non-violations of the Bell-type inequalities for full factorisability and the Svetlichny inequalities for partial factorisability (sections 5.2.1 and 5.4.1 respectively).

The investigation for the case of full factorisability, i.e. (non-)violations of Bell-type inequalities, has been performed for all possible systems (N sub-systems with each a Hilbert space of dimension d) and for most measurement configurations (N, m, d).

Not surprisingly the fully separable states do not violate any Bell-type inequality whereas the fully entangled GHZ-states maximally violate them. However, noteworthy is the fact that the ratio of violation for these fully entangled states increases for both particle number N and spin number j. Thus, for the Bell inequalities in the macroscopic limit we see a divergence between the classical and the quantum mechanical formalism. Further even more noteworthy is the fact that the fully separable states are not the only states non-violating any Bell inequality. Some entangled states exist that have a local HV-model for all orthodox measurements and will thus not violate a Bell inequality. These are the Werner states. This phenomenon has revealed that factorisability (of local hidden variable predictions) and separability (of quantum states) are quite distinct notions that cannot be identified, except for the special case of pure two-particle states. This gives the following conclusion: The requirement of having a fully separable quantum description of the two or more subsystems is a more stringent condition than the requirement of admitting any possible local hidden variable model.

The entanglement in the Werner states can not be revealed using a Bell inequality when subjected to orthodox measurements and is therefore said to be 'hidden'. But surprisingly it can be revealed using a Bell inequality when performing generalized quantum measurements such as sequential measurements that can be modeled using POVMs. This the so-called phenomenon of 'revealing hidden entanglement'. This will be treated in the next chapter.

The extension to partial factorisability and the corresponding Svetlichny inequalities and partial local HV-theories has been performed in section 5.4. Here the known quantum mechanical violations and non-violations of the Svetlichny inequalities are presented for the single measurement configuration $(N, 2, 2)$. Again the fully entangled GHZ states give maximal violations and the fully separable states non-violations. Furthermore, because violation of the Svetlichny inequalities is sufficient for full entanglement, all non-fully entangled states will not give a violation. However, analogously to the bi-partite Werner states, some fully entangled states cannot give any violation (this is the set of states ρ_S^N). This implies that partial factorisability (of partial local hidden variable predictions) and partial separability (of quantum states) are quite distinct notions that should not be identified.

The Svetlichny inequalities are only a necessary and not sufficient set of inequalities for partial factorisability to hold. Nevertheless, just like in the case of full factorisability where such a set exists, I believe such a set to also exist for partial factorisability. This leads to the following conjectured conclusion: The requirement of having a partially separable quantum description of the three or more subsystems is a more stringent condition than the requirement of admitting any possible partial local hidden variable model.

In section 5.3 all the results obtained in this chapter and the previous two about the relationship of the quantum mechanical state space with the hidden variable structure for full factorisability, have been presented in implication diagrams. This summarizes most results and conjectures for the case of full factorisability.

In section 5.5 all results obtained about the relationship of the quantum mechanical state space with the hidden variable structure for case of partial factorisability have been presented in implication diagrams. Compared to the case of full factorisability this is very non-detailed. However, the results address the fundamental question of whether Nature somehow limits the number of particles that can be fully entangled, that is to say whether or not some form of partial separability holds.

Lastly, in order to continue the classification of the quantum state space that has been performed in all previous chapters, the newly distinguished quantum states of this chapter are summarized in section 5.6.

Chapter 6

Local Realism and General Quantum Measurements

The question of which quantum states admit a (partial) local hidden variable model has been investigated in the last two chapters. There the following was discussed. For pure entangled quantum states of two or more particles observables can be found that will violate a Bell type inequality upon measurement. Thus no local HV model exists for these states; The only local states are the product states. However for mixed states the problem becomes more complicated. Unexpectedly it is not the case that the only mixed states that do not violate a Bell-type inequality are the mixtures of product states (i.e. separable states). This was first shown by Werner who presented the existence of a class of mixed states which are entangled but nevertheless admit a LHV model.

However Werner had considered a restrictive set of measurements, namely the single (i.e. non-sequential) Von Neumann measurements. Popescu [54] was the first to note this and has furthermore shown that most of the Werner-states exhibit violation of the CHSH inequality if sequences of orthodox measurements are taken into account [53] This exposure of non-locality, the so-called *hidden non-locality*, involves non-orthodox quantum measurement procedure, namely sequences of orthodox measurements in which the first measurement acts as a selection procedure for the second measurement.

After Popescu discovered this procedure to 'reveal the hidden entanglement' other such procedures were found. Peres [61] used collective local measurements on a large number of the same Werner states to show violation of the CHSH inequality. And Gisin [102] used a procedure called local filtering, i.e. independent interaction of the two particles with two environments, to show that a specific set of two particle states can be made to violate a CHSH inequality, whereas for orthodox single measurements this would not occur. This has broadened the class of quantum states that have statistical properties that violate local realism.

These three procedures, which will be treated in this chapter in section 6.1, show that the extension of only orthodox measurements to more general types of measurements puts the question of which quantum states are non-local into new perspective: "When is a quantum state (non-)local? Does one have to consider only orthodox or also general measurement procedures?" These questions form the motivation for this chapter to study more general measurements and their implications for local realism.

In order to apply the hidden variable formalism to these general quantum measurements the Quantum-criterium of section 4.2.1 has to be changed. The local HV model has to reproduce not only the orthodox measurements but also the specific types of general measurements. This extension of the Quantum-criterium will be discussed in section 6.2 after which the HV-models for more general measurements will be explicitly considered.

This chapter contains much work that is still in progress and therefore a lot of open questions exist. Some of them will be treated in the conclusion.

6.1 Revealing Hidden Non-locality

In this section I present the basic ideas behind three different ways of 'revealing hidden non-locality', i.e. of violating a Bell-type inequality using some sort of general measurement scheme for states that show no violation when using only orthodox measurements.

6.1.1 Sequential Measurements

Consider the Werner states on the Hilbert spaces $\mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$ with $\mathcal{H}^{(1)} \cong \mathcal{H}^{(2)} \cong \mathbb{C}^d$ where each system has equal dimension d,

$$\rho_W = \frac{1}{d^3}\mathbb{1} \otimes \mathbb{1} + \frac{2}{d^2}P^{anti} = \frac{1}{d^3}\mathbb{1} \otimes \mathbb{1} + \frac{1}{d^2}\sum_{i<j;i,j=1}^{d} |\,\phi_{i,j}\rangle\,\langle\,\phi_{i,j}|\,. \tag{6.1}$$

Here P^{anti} is the projection onto the completely anti-symmetric subspace of $\mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$ and $|\,\phi_{i,j}\rangle$ is the 'spin-1/2 singlet state'

$$|\,\phi_{i,j}\rangle = \frac{1}{\sqrt{2}}(|\,i\rangle_1\,|\,j\rangle_2 - |\,j\rangle_1\,|\,i\rangle_2), \tag{6.2}$$

where $\{|\,i\rangle_1\}$, $\{|\,i\rangle_1\}$ are orthonormal bases in $\mathcal{H}^{(1)}, \mathcal{H}^{(2)}$ respectively. Recall that Werner has constructed a local HV-model for orthodox measurements for these states and that therefore they do not violate the CHSH-inequality using orthodox measurement procedures.

The interesting feature Popescu [53] discovered is that when we perform local measurements of the form $\hat{A} = \hat{R} \otimes \hat{\mathbb{I}}$ and $\hat{B} = \hat{\mathbb{I}} \otimes \hat{R}$ where $\hat{R}$ is a projector on a two dimensional subspace of $\mathbb{C}^2$, $\hat{R} = |\,1\rangle\,\langle\,1| + |\,2\rangle\,\langle\,2|$, we get correlations in a subensemble that violate the CHSH inequality. Popescu showed that the subensemble for which both $\hat{A}$ and $\hat{B}$ yield the outcome 1, given by the collapsed density operator

$$\rho_W' = \frac{\hat{A}\hat{B}\rho_W\hat{A}\hat{B}}{\mathrm{Tr}(\rho_W\hat{A}\hat{B})}, \tag{6.3}$$

violates the CHSH inequality for $d \geq 5$ for an appropriate set of local orthodox measurements. Thus there are local observables whose correlations in this new state can no longer be described by a local HV-model. In conclusion, sequences of two ideal measurements, where the first measurement acts as a state selecting procedure for the second measurement, can reveal the hidden entanglement.

Because the observables leading to a violation of the CHSH inequality used by Popescu commute with $\hat{A}$ and $\hat{B}$, the time sequences of measurements can be described by a single POVM[1], and thus Werner's local HV-model applies to it. However, "the model thus violates causality: later measurements influence preceding ones [44]." Since such a model does not capture the physical idea that there are no actions into the past, Popescu [53] and Mermin [40] required that a local hidden variable model must satisfy apart from the locality condition the causality condition that initial measurements do not depend upon what measurements are later performed. This has resulted in the construction of a *local causal hidden variable model* (LCHV) by Teufel *et al.* [44] in which they explicitly required this causality condition to hold for any possible local HV-theories that model the outcomes of sets of sequential orthodox measurements. This model will be treated in the next section.

6.1.2 Collective Measurements

Peres [61] used a measurement scheme to reveal the hidden entanglement from 2×2 Werner states using collective measurements.[2] He showed that if the density operators ρ_W obey the CHSH inequality, the collective state $\rho_W \otimes \rho_W \otimes \rho_W \otimes \rho_W \otimes \dots$ will violate that inequality when measuring suitably chosen observables.

The protocol Peres used is a sort of distillation protocol describable by LOCC and goes as follows. Each one of the two observers has N particles, one particle from each Werner pair. They subject their N particle state to suitably chosen local unitary transformations $\hat{U}$ and $\hat{V}$. Then, they test whether each one of the particles labeled $2, 3, \dots, N$ has spin 'up'. If this is not the case, the experiment is considered to have failed and has to be performed over again. For simplicity I will further consider the case that $N = 3$. The result of the unitary transformation $\hat{U}$ and $\hat{V}$ on a three particle state $\rho_W \otimes \rho'_W \otimes \rho''_W$ is $(\hat{U}\otimes\hat{V})(\rho_W \otimes \rho'_W \otimes \rho''_W)(\hat{U}^\dagger \otimes \hat{V}^\dagger)$. The matrix elements of the $\hat{U}$ matrix satisfy:

$$\sum_{mm'm''} U_{\mu\mu'\mu'',mm'm''} U^*_{\lambda\lambda'\lambda'',mm'm''} = \mathbb{1}. \tag{6.4}$$

A similar result holds for the $V_{\nu\nu'\nu'',n'n''n'''}$ matrix elements.

Peres has shown that the selective procedure to keep only those transformed states that have spin 'up' for particles $2, 3, \dots, N$ places such restrictions on the rows of the matrix of $\hat{U}$ that effectively on the left hand side of Eq.(6.4) only two unknown vectors U_0 and U_1 remain. Each has 2^N components labeled $mm'm'''$ and are of unit norm and are mutually orthogonal. Likewise the second observer has two vectors V_0 and V_1. The problem Peres solved was to optimize these vectors so as to violate the CHSH inequality for an optimal set of observables A, A', B, B'. This optimization procedure is rather complicated and will not be shown here. The result however is that a violation of the CHSH inequality can be obtained for

[1] Questions about actual measurability of the observable corresponding to the POVM will not be considered.

[2] For completeness, Bennett *et al.* [101] have shown that *all* Werner states ($N \times N$, $N = 2, 3, \dots$) can be distilled, and therefore made to violate a CHSH inequality using collective measurements.

the state $\rho_W \otimes \rho'_W \otimes \rho''_W$ where ρ_W admits a local HV model (a Werner model) for orthodox measurements.

According to Peres this has he following implication. "Even if a local HV model is possible for the statistics of a single pair of particles, there may be no extension of such a model is possible when several pairs are tested collectively, provided that the particles held by each observer are allowed to interact locally before they are tested."[61] This example by Peres motivates the extension, performed in the next section, of the hidden variable formalism to collective measurements.

6.1.3 Local Filtering

Gisin [102] use a technique called local filtering to reveal the hidden entanglement of a specific set of two spin-$\frac{1}{2}$ systems. He takes certain spin-$\frac{1}{2}$ mixed states, similar to the Werner states, consisting of a fraction of singlet states and a fraction of pure product states. Further he uses so-called dichroic elements as filtering elements such that the state after the filtering, i.e. after passage through the dichroic element, contains a larger fraction of the singlet state. The dichroic elements are for example in the case of photons polarizing optical fibers or transmission at the Brewster angle. Gisin uses the polarizing elements in his photon example.

These filters act independently and locally on each of the two particles. The effect of the filtering process is the following. It can be viewed as selective absorption. The states before filtering are shown not to give a violation of the CHSH inequality, but after filtering the fraction of singlet states is increased such that the CHSH-inequality indeed can be violated. Thus this filtering reveals the hidden entanglement.

Because the filtering process can also be viewed as selective absorption it can be treated as a generalized measurement, i.e. describable by a POVM: the combination of a fixed filter and an orthodox measurement constitutes a generalized measurement [104]. This motivates the further study of the hidden variable formalism in the case of generalized quantum measurements. It is performed in the next section.

6.2 Extended Local HV-models

Although from the view of quantum mechanics all previous measurement schemes are describable by local operations and classical communication (LOCC), from the view of a hidden variable theory distinctions need to be made. Each different measurement scheme gives different requirements for local HV-theories that try to model the outcomes of these measurments. Further, in order to extend the hidden variables program of chapter 4 to deal with the special measurement procedures of the previous section and with any other more general measurements, the Quantum-criterium of section 4.2.1 that deals only with orthodox measurements must be adjusted. This definition of the Quantum-criterium does not apply to local HV-theories for non-orthodox quantum measurements. Here I want to change the Quantum-criterium so as to allow a local HV-theory for more general quantum measurement procedures described by POVMs, collective and sequential measurements.

A multitude of Quantum-criteria emerge depending upon what sort of measurements one wants to model with the HV-theory. Below I list the different generalized observables and possibilities for measurement protocols.

1. Observables and their Representation as Operators.
   - Orthodox Measurements. Observables represented as a projection valued measure (PVM). See section 2.7.1 for the definition and characteristics.
   - Generalized Measurements. Observables represented as a positive operator valued measure (POVM). See section 2.7.2 for further definition and characteristics.
2. Measurement protocols.
   - Sequential Measurements. Each measurement in the sequence acts on the state that resulted from the previous measurement. This allows for selective procedures. It introduces a temporal aspect: the time ordering of the sequences of measurement.[3]
   - Collective Measurements. Instead of measuring the state ρ one performs measurements on the single collective state $\rho \otimes \rho \otimes \rho \otimes \rho \otimes \ldots$. This allows for distillation.
3. Local Operations and Classical Communication.
   - LOCC. On a composed system consisting of two subsystems LOCC are any completely positive linear and trace-preserving map of the density operator of the first subsystem that leaves unchanged the state of the second subsystem. Using local POVMs and classical communication one can perform sequential measurements and non-local selective procedures. For example, depending on the outcome of local measurements and classical communication each party can select a subset from their ensemble of states. See also section 3.1.4 for the definition of LOCC.
   - CLOCC. Using LOCC and collective measurements. This allows for the the most general local measurement protocols including non-local selection (using the classical communication) and distillation.

A local HV-theory for only orthodox quantum measurements (not collective, not sequential, and not selective measurements) was discussed in chapter 2. It has to obey the Quantum criterium of section 4.2.1. Local HV-theories for the other measurement schemes of the above listing and combinations of them are discussed below. This has not been thoroughly investigated yet, and thus presentation is not a complete survey nor is it very detailed.

6.2.1 Local HV-theory for Orthodox and Sequential Measurements

Because a time ordering appears in the sequential measuring process an extra condition of causality will be required of the local HV-model that models these

[3] For simplicity, I will ignore any appropriate special relativistic terminology.

sequential and orthodox measurements. The model must capture the physical idea that there are no actions into the past. This is the point of view that a physically reasonable local hidden variable model must satisfy apart from the locality condition the causality condition that initial measurements do not depend upon what measurements are performed at a later time.

Teufel *et al.* [44] use this point of view to construct a *local causal hidden variable model* (LCHV) in which they explicitly required this causality condition to hold for any possible local HV-theories that model the outcomes of sets of sequential orthodox measurements.

The model of Teufel *et al.* [44] uses the usual hidden variable space Λ and a set of random variables X such that for any time ordered sequence $(t_1 < \ldots < t_n)$ of observables $A^1(t_1), \ldots A^n(t_n)$, each with spectrum $s(A^i)$, there is a corresponding random variable, a function

$$X_{A^1(t_1),\ldots A^n(t_n)} \ : \ \Lambda \longrightarrow s(A^1) \times \ldots \times s(O^n) \quad \subset \mathbb{R}^n, \tag{6.5}$$

whose distribution represents the quantum mechanical distribution of predictions for ideal measurements of the observables $A^1(t_1), \ldots A^n(t_n)$:

$$\mathbb{P}(X_{A^1(t_1),\ldots A^n(t_n)} = (a_1, \ldots , a_n)) \ = \ \mathrm{Tr}[P^n_{a_n} \ldots P^1_{a_1} \rho P^1_{a_1} \ldots P^n_{a_n}]. \tag{6.6}$$

Here a_i are the possible measurement results and $P^n_{a_n}$ is the projection operator onto the eigenstate of the observable A^n corresponding to the eigenvalue a_n. [4]

The causality condition is now represented as:

$$X^{A^n_{(t_n)}}_{A^1(t_1),\ldots A^n(t_n)} = X_{A^1(t_1),\ldots A^{n-1}(t_{n-1})}, \tag{6.7}$$

where $X^{A^n_{(t_n)}}_{A^1(t_1),\ldots A^n(t_n)}$ is the random variable describing the outcome of the first $(n-1)$ measurements which, in general, depends on the later measurement $A^n(t_n)$.

The locality condition is the same as used for the local HV model for orthodox measurements:

$$X_{A^1(t_1),\ldots A^n(t_n),B^1(t_1),\ldots B^n(t_n)} = (X_{A^1(t_1),\ldots A^n(t_n)}, X_{B^1(t_1),\ldots B^n(t_n)}). \tag{6.8}$$

Here the observables A^i and B^j are spatially separated.

Then a *local causal hidden variables model* (LCHV) is a HV-model that is both local and causal in the above defined sense. Teufel *et al.* now use this model to investigate different types of non-locality. They present the following conjecture which they can neither prove nor disprove:

Conjecture 6.2.1. *For $d > 2$ no entangled density operator on $\mathbb{C}^d \otimes \mathbb{C}^d$ admits an LCHV.*

[4] Although this requirement of Eq. (6.6) marks a deterministic HV-theory the extension to the more general stochastic HV-theory can be performed and shows no new relevant features. In fact Teufel *et al.* perform this extension.

Preselection of a Subensemble

Sequential measurements allow for the possibility of locally preselecting a subensemble upon which further measurements are to be performed. As was seen in the Popescu example of section 6.1.1 this preselecting allows for the revealing of hidden entanglement. However to formally address non-locality issues in case of local preselection, a local hidden variables description is needed. This was performed by Zukowski *et al.* [104] and will here be outlined.

Consider an experiment on a two particles system of two consecutive measurements performed on each particle. Denote these measurements as A_1, A_2, B_1 and B_2, with possible outcomes a_1, a_2, b_1 and b_2. The locality requirement of the HV-model for these measurements then becomes

$$\mathbb{P}_{A_1,A_2,B_1,B_2}(a_1, a_2, b_1, b_2) = \int_\Lambda \mathbb{P}_{A_1,A_2}(a_1, a_2|\lambda)\mathbb{P}_{B_1,B_2}(b_1, b_2|\lambda)\mu(\lambda)d\lambda, \quad (6.9)$$

with Λ the space of hidden variables λ and $\mu(\lambda)$ the probability distribution of λ.

Because of the sequential procedure one more requirement becomes relevant. This is the requirement of causality. In general the choice of the second observable A_2 (and B_2) is made *objectively after* the measurement of A_1 (and B_1). The physically reasonable requirement of *causality* then implies that the probabilities $\mathbb{P}_{A_1,A_2}(a_1, a_2)$ and $\mathbb{P}_{B_1,B_2}(b_1, b_2)$ cannot depend on respectively A_2 and B_2.

Denote now by χ the set of conditions $\{A_1, B_1, a_1, b_1\}$ given by the first measurement. Each one of these conditions allows for preselection of a specific state upon which the second measurement is performed. Then the conditional probabilities $\mathbb{P}^\chi_{A_2,B_2}(a_2, b_2) \equiv \mathbb{P}_{A_1,A_2,B_1,B_2}(a_2, b_2|a_1, b_1)$ of the model of Eq. (6.9) for the second measurement are of the following form [104]:

$$\mathbb{P}^\chi_{A_2,B_2}(a_2, b_2) = \int_\Lambda \mathbb{P}^\chi_{A_2}(a_2|\lambda)\mathbb{P}^\chi_{B_2}(b_2|\lambda)\mu^\chi(\lambda)d\lambda \quad (6.10)$$

Note that $\mu^\chi(\lambda)$ is independent of the observables $A_2,\ B_2$ and independent of the outcomes $a_2,\ b_2$. The conditional probabilities thus acquire the typical form for the standard local HV-theories (compare with Eq. (4.19) of section 4.2.3). Thus these must satisfy the Bell inequalities.

This has the following results. Local realism in conjunction with causality implies that any subensemble preselected by certain specific local measurements and a specific unique set of their results (denoted by χ) is describable by a local HV-model. Further the existence of a local HV-model for a preselected ensemble is a necessary condition for the existence of a local HV-model for the full ensemble. Zukowski *et al.*. [104] formulate this as follows: "If a subensemble does not admit a local hidden variables description, the full ensemble does not either. In simple words, the existence of a model given by Eq.(6.10) is a necessary condition for the existence of a model of Eq. (6.9)."

Thus if a certain preselected subensemble violates a Bell inequality then this implies that the original ensemble (i.e. state) does not allow any local realistic description of sequential measurements. The possibility of a local causal HV-model for joint probabilities of sequences of measurements can therefore be checked indirectly by using the much more easy task of checking whether some conditional probabilities of single measurements allow the model.

6.2.2 Local HV-theory for POVM Measurements

The extension of a local HV-theory from PVM measurements to POVM measurements (no collective and no sequential measurements) has been performed by Barrett [100]. He explicitly constructs a local HV model for generalized measurements (called a LHVPOV-model) for some specific class of entangled density operators, a set of generalized Werner states. The method he uses is to first create the model for POVM elements proportional to projection operators, and then show that this model implies the existence of a model for all POVM measurements.

The explicit model will here not be given, but the question whether other entangled states might admit an LHVPOV gives an interesting result. Barrett [100] showed that an LHVPOV model for a state ρ_1 implies the existence of an LHVPOV model for the state ρ_2 if the states are related to each other in the following way:

$$\rho_2 = \sum_{ij} M_i \otimes N_j \rho_1 M_i^\dagger \otimes N_j^\dagger, \tag{6.11}$$

where $\sum_i M_i M_i^\dagger = \mathbb{1}$ and $\sum_i N_j N_j^\dagger = \mathbb{1}$. In other words, a LHVPOV model for ρ_2 exists if it can be obtained by local operations and non-selective classical communication from another state admitting such a model.

The LHVPOV model Barrett constructed for the set of generalized Werner states proved the following conjecture to be false.

Conjecture 6.2.2. *Any entangled state will violate some Bell-type inequality if the two parties can perform single (i.e. non-sequential) POVM measurements on individual copies of the state.*

Then a natural conjecture is the following:

Conjecture 6.2.3. *Any entangled state will violate some appropriate Bell-type inequality if the two parties can perform arbitrary sequences of POVM measurements on individual copies of the state.*

This conjecture is the same as conjecture 6.2.1 of Teufel *et al.*. but now for the case of POVM measurements. It will be investigated in the next subsection.

6.2.3 Local HV-theory for all LOCC

The inclusion of all LOCC operations in an HV-model, i.e. to include any sequential and selective measurements (excluding collective measurements), gives the following extension of the model for sequential measurements of Eq.(6.6). A family of generalised observables $\{\mathcal{E}_{\gamma_i}\}$ is used that give the POVM operations R_{γ_i} for the spectrum $\{\gamma_i\}$. See section 2.7.2 for this procedure.

Equation (6.6) for the quantum mechanical probabilities is then replaced by:

$$\mathbb{P}(X_{\mathcal{E}^1(t_1),\ldots\mathcal{E}^n(t_n)} = (\gamma_1, \ldots, \gamma_n)) \;=\; \mathrm{Tr}[R^n_{\gamma_n} \ldots R^1_{\gamma_1} \rho (R^1_{\gamma_1} \ldots R^n_{\gamma_n})^\dagger]. \tag{6.12}$$

The locality condition of Eq.(6.8) and the causality condition of Eq.(6.7) are unchanged.

Using such a model, called a local causal hidden variables model for generalized measurements (LCHVG)[44], the following natural conjecture arises.

Conjecture 6.2.4. *For $d > 2$ no entangled density operator on $\mathbb{C}^d \otimes \mathbb{C}^d$ admits an LCHVG.*

As yet this conjecture is neither proved nor disproved.

6.2.4 Local HV-theory for all Collective LOCC (CLOCC).

In the Peres example of revealing hidden non-locality in section 6.1.2 measurements on $\rho \otimes \rho \otimes \rho \otimes \ldots$ were considered and not just on the single state ρ. These collective measurements were shown to reveal new aspects of the non-locality of quantum states. A natural extension would then be to require besides the normal LOCC also that any HV-model must be able to reproduce collective measurements. However this has as yet not been explicitly formalized.

Nevertheless a first result is the following. The distillation process of section 3.3 is an example of a collective measurement protocol. Because of this a local HV-theory for collective LOCC should at least be able to model outcomes of distillation protocols. Future research is needed to fully see what collective measurements can or cannot say about non-locality.

6.3 Conclusion and Summary

In this chapter local HV-theories for more general types of measurement than the orthodox are discussed. The motivation for this are three examples of revealing hidden non-locality using sequential, POVM and collective measurements. This revealing has broadened the class of quantum states that have statistical properties that violate local realism. In order to apply the hidden variable formalism to these general quantum measurements, the Quantum-criterium of section 4.2.1 is changed: the local HV-model has to reproduce not only the orthodox measurements but also the specific types of general measurements.

In section 6.2 the embedding of different measurement protocols in local HV-models is discussed. Sequential measuring introduces a time ordering which results in a causality condition stating that future measurements do not influence earlier ones. Teufel *et al.*. [44] have explicitly formulated this causality condition and constructed a local causal HV-model (LCHV). Furthermore, sequential measuring allows for preselection. Zukowski [104] analysed this. The result is that the existence of a local HV-model for a preselected ensemble is a necessary condition for the existence of a local HV-model for the full ensemble. Then the possibility of a local causal HV-model for joint probabilities of sequences of measurements can be checked indirectly by using the much more easy task of checking whether some conditional probabilities of single measurements allow the model.

The extension to POVM measurements and further to local actions and classical communication (LOCC) has resulted in the specification of a local causal HV-model for generalized measurements (LCHVG). The following conjecture which is as yet neither proved nor disproved then arises: For $d > 2$ no entangled density operator on $\mathbb{C}^d \otimes \mathbb{C}^d$ admits an LCHVG. It would be an interesting open problem to try to prove this conjecture.

Let's go back to the question raised in the introduction of this chapter. "When is a quantum state local?" The obvious answer is that a quantum state is local if a local HV theory exists which is valid for all results of all possible local actions. Equivalently, a quantum state is local when it cannot be made to violate a Bell-type inequality that is obtained from a local HV-theory valid for all possible local actions. Here local actions are all (sequences of) LOCC. Thus the argument for taking an original unprocessed entangled state to intrinsically possess non-local (as opposed to merely entangled) correlations is a violation of a Bell-type inequality using (sequential) LOCC.

One could also include collective measurements (CLOCC) so as to violate a Bell-type inequality. Peres used this in his example to reveal hidden entanglement from the Werner states. However a critique about the inclusion of collective measurements into the set of local actions that a HV-model must reproduce is the following. One measures the state $\rho^N = \rho_1 \otimes \ldots \otimes \rho_N$ and not ρ. Thus one could argue that if collective measurements on N copies of a state ρ are needed to reveal non-locality then it is the state ρ^N that is non-local rather than ρ [86].

As an open problem note that only the HV-theories for full factorisability have been treated in this chapter. What about the extension to general measurements in partial local HV-theories (PLHV)? So far no result have been obtained, although a motivation for future research in this direction would be the following. Recall the fully entangled states ρ_S^N of the previous chapter (Eq.(5.40). which cannot be made to violate a Svetlichny inequality for orthodox measurements. Perhaps using general measurements they can be made to violate a Svetlichny inequality? This would amount to revealing the full entanglement of these quantum states ρ_S^N using a Svetlichny inequality obtained from a partial local HV-model.

Chapter 7

Conclusion, Results and Summary

In this chapter I will give a summary of the previous chapters focussing on the conclusions and results that together constitute the core of this thesis.

In this thesis local hidden variable theories have been used as a means for investigating quantum mechanics and *vice versa* by discussing some currently known results and by adding some new ideas and results. As preliminary information the basic mathematical structure of quantum mechanics was presented in chapter2. Three different sets of postulates were obtained. The first for pure states and projective measurements, the second included the extension to mixed states. This completed the structure of orthodox quantum mechanics. The third set of postulates captured the extension of projection valued measures (PVM) to positive operator valued measures (POVM). This gives the set of postulates of quantum mechanics for general measurements.

The first novel result obtained in this thesis is the following. Because quantum mechanics primarily deals with measurement outcomes it became necessary to give the standard formulation of measurement compatibility (i.e. simultaneous measurability) of observables. We have seen that in the standard account measurement compatibility was identified with commutativity. However, I have criticized this identification and have argued that commutativity is not sufficient for measurement compatibility using a simple example that was inspired by Harvey Brown [82]. An interesting open problem, not investigated here, is to find out what mathematical characterization captures the physical notion of measurement compatibility in a satisfactory way.

In chapter 3 I have considered quantum entanglement. An entangled state is defined as a non-separable state. Therefore the separability properties of density operators are discussed. The partial transpose criterium is shown to give a necessary criterium for separability, and for small tensor product Hilbert spaces it gives a sufficient criterium as well. The structure of the bi-partite, tri-partite and N-partite entangled state space has been investigated and specific distinctions such as maximal and full entanglement have been made. The distillation of a collection of entangled states to the maximally entangled bi-partite has been discussed. states. The distillability and separability properties of quantum states have been explicitly related to each other, and the implicative connections have been shown in specific figures (figure 3.4 and 3.5).

It was found that separability implies positive partial transposition, although the converse is not true for all states. Positive partial transposition in turn implies non-distillability. Whether the converse holds –i.e. whether non-distillability implies positive partial transpose– is not yet known. However, for bi-partite two-dimensional systems all three concepts imply each other.

In order to confront quantum mechanics and the feature of entanglement to the structure of hidden variables theories, I discussed the incompleteness problem of quantum mechanics in chapter 4. The discussion of this problem –whether or not quantum mechanics provides a complete physical theory– served as a stepping stone for the study of hidden variables theories as theories that could possibly be more complete than quantum mechanics itself.

The derivation of the Bell-inequalities and the Bell-theorem were presented as preliminary work for the remainder of the thesis. In this remainder more complex systems were studied than the bi-partite spin-1/2 systems which were the paradigmatic systems for the original Bell-theorem and all its initial variations on the same theme.

More complex bi- and tri-partite systems provide further *Gedankenexperiments*, the so-called Bell-theorems without inequalities and the algebraic theorems. As examples the Bell-theorem without inequalities of Hardy and the algebraic proof of Greenberger, Horne and Zeilinger (GHZ) have been discussed. I have compared these new Bell-theorems to the original Bell-theorem for logical strength and experimental testability. The algebraic Bell-theorem of GHZ has been argued to be the logically most strong theorem. It requires a minimum of quantum structure to arrive at a contradiction with local realism. However, from an experimental point of view, I have argued the original Bell-theorem to be superior because it can be most easily experimentally implemented. The Bell-theorem without inequalities of Hardy and the algebraic proof of GHZ were in fact argued –contrary to claims of the originators– to not give an 'all or nothing' situation that can be decided in a single experimental run because of neglect of measurement compatibility. This is in fact the same criticism as was given in chapter 2 about the identification of commutativity with measurement compatibility.

The extension to N-partite systems has resulted in the necessary distinction between the specific locality-hypotheses of full and partial factorisability. The Bell-Klyshko N-partite Bell-type inequalities for full factorisability were discussed as well as the extension to complete sets (i.e. necessary and sufficient sets) of Bell-type inequalities. The extension to multi-partite systems for which the specific locality hypothesis of partial factorisability is required to hold, has been shown to result into a new type of hidden variable theories, the so-called partial local hidden variable theories (PLHV). As a result the generalized Svetlichny inequalities were derived (together with George Svetlichny) and they were shown to be necessary inequalities for any PLHV to hold.

The three types of inequalities – the Bell-inequalities, the N-partite Bell-Klyshko inequalities for full separability and the Svetlichny inequalities for partial separability – were all confronted with the feature of quantum entanglement. As a result I have shown that that these inequalities give experimentally accessible sufficient conditions for respectively bi-partite and full N-partite entanglement. These inequalities thus serve a dual purpose. As tests for the possibility of certain local hidden variables models and as tests for entanglement.

In order to further investigate the quantum mechanical state space by means of local hidden variable theories, chapter 5 has been largely devoted to quantum mechanical violations and non-violations of the Bell-type inequalities in the case of full factorisability and of the Svetlichny inequalities in the case of partial factorisability.

The discussion for the case of full factorisability, i.e. (non-)violations of Bell-type inequalities, has been performed for all possible systems (M sub-systems with each a Hilbert space of dimension d) and for all measurement configurations (N, m, d). For all these cases the following two central questions were discussed:

1. What is the set of Bell-correlated states, i.e. violating a Bell-type inequality?

2. What states violate the different inequalities maximally?

These questions are far from completely answered in of the cases discussed above. Nevertheless some definite results have been discussed of which the most important are the following.

Not surprisingly the fully separable states do not violate any Bell-type inequality whereas the fully entangled GHZ-states maximally violate them. Further for the case of the measurement configurations $(2, 2, 2)$ all pure entangled states violate the CHSH inequality and it is violated maximally iff the state is maximally entangled. Noteworthy is the fact that the ratio of violation for the fully entangled states of N-partite inequalities increases for particle number N and remains for increasing spin number j. Thus, we see a divergence between the classical and the quantum mechanical formalism for increasing particle number. Even more noteworthy is the fact that the fully separable states are not the only states non-violating any Bell inequality. Some entangled states exist that have a local hidden variables model for all orthodox measurements and will thus not violate a Bell-type inequality. These are the Werner states. This phenomenon has revealed that factorisability (of local hidden variable predictions) and separability (of quantum states) are quite distinct notions that cannot be identified, except for the special case of pure two-particle states. One may thus conclude the following: The requirement of having a fully separable quantum description of the two or more subsystems is a more stringent condition than the requirement of admitting any possible local hidden variable model.

The extension to partial factorisability and the corresponding Svetlichny inequalities which are derived from partial local hidden variables theories has been performed in section 5.4. Here the known quantum mechanical violations and non-violations of the Svetlichny inequalities are presented for the single measurement configuration $(N, 2, 2)$. Again the fully entangled GHZ states give maximal violations and the fully separable states non-violations. Furthermore, because violation of the Svetlichny inequalities is sufficient for full entanglement, all non-fully entangled states will not give a violation. However, analogously to the bi-partite Werner states, some fully entangled states cannot give any violation (this is the set of states ρ_S^N of Eq. (5.40). This implies that partial factorisability (of partial local hidden variable predictions) and partial separability (of quantum states) are quite distinct notions that should not be identified.

The Svetlichny inequalities are only a necessary and not sufficient set of inequalities for partial factorisability to hold. Nevertheless, just like in the case of full factorisability where it was shown that such a complete set exists, I believe such a set to also exist for partial factorisability. This leads to the following conjectured conclusion: The requirement of having a partially separable quantum description of the three or more subsystems is a more stringent condition than the requirement of admitting any possible partial local hidden variable model.

Throughout this thesis the investigation of quantum mechanics using local hidden variable theories has resulted in a classification of different quantum states. This classification is presented at the end of chapter 2, 3, 4 and 5 and was performed, (i) through the formalism, (ii) through extending the formalism, (iii) through entanglement properties and aspects of quantum information, (iv) through factorisability (full and partial), (v) through (non)-violations of Bell-type inequalities.

As mentioned earlier, the entanglement in the Werner states can not be revealed using a Bell inequality when subjected to orthodox measurements. It is therefore said to be 'hidden'. But surprisingly it can be revealed using a Bell inequality when performing generalized quantum measurements such as sequential measurements that can be modeled using POVMs. This the so-called phenomenon of 'revealing hidden entanglement' that is a central theme in the last chapter, chapter 6. Three examples of revealing hidden non-locality –using sequential, POVM and collective measurements– are discussed. They have broadened the class of quantum states that have statistical properties that violate local realism. Thus in order to answer the question of which quantum states will violate a Bell-type inequality, generalized measurements have to be included as well. Accordingly chapter 6 deals with local hidden variables theories for more general types of measurement than the orthodox ones. In order to apply the hidden variable formalism to these general quantum measurements, the Quantum-criterium is changed: the local hidden variables model has to reproduce not only the orthodox measurements but also the specific types of general measurements.

The embedding of different measurement protocols in local hidden variables models is discussed. The extension to sequential measurements, local filtering and further to local actions and classical communication (LOCC) has resulted in the specification of a local causal hidden variables model for generalized measurements (LCHVG). The following conjecture which is as yet neither proved nor disproved then arises: For $d > 2$ no entangled density operator on $\mathbb{C}^d \otimes \mathbb{C}^d$ admits an LCHVG. It would be an interesting open problem to try to prove this conjecture.

Finally, the question "When is a quantum state local?" has the obvious answer that a quantum state is local if a local hidden variables theory exists which is valid for all results of all possible local actions. Or equivalently, a quantum state is local when it cannot be made to violate a Bell-type inequality that is obtained from a local hidden variables theory valid for all possible local actions. Here local actions are all (sequences of) LOCC.

One can also include collective measurements into the set of local actions that a hidden variables model must reproduce. However, I have criticized this as follows. One measures the state $\rho^N = \rho_1 \otimes \ldots \otimes \rho_N$ and not ρ. Thus if collective measurements on N copies of a state ρ are needed to reveal non-locality then it is the state ρ^N that is non-local rather than ρ [86].

Because the inclusion of generalized measurements in hidden variables theories has only been performed for hidden variables theories with full factorisability, the inclusion of generalized measurements for hidden variables theories with partial factorisability is still an open problem. A motivation for future research in this direction is the following. Recall that fully entangled states exist that cannot be made to violate a Svetlichny inequality for orthodox measurements. Perhaps using general measurements they can be made to violate a Svetlichny inequality. This would amount to revealing the full entanglement of these multi particle quantum states using a Svetlichny inequality obtained from a partial local hidden variables model.

As a final remark to conclude this thesis, let me recall the following remark given in the introduction. "Whereas in the late Eighties there was hardly any difference between entangled states and states violating a Bell inequality, we have a much more subtle discrimination nowadays." [105] The thing to have learned from this remark is the simple but pround insight already mentioned in the introduction of this thesis: There are two issues which are quite separate: Which states are entangled and which states have non-local characteristics? The first question asks about the mathematical structure of quantum mechanics, the second question asks about the physical structure of local hidden variables theories. Good understanding of this difference and when it applies is essential to any further investigations and breakthroughs. I hope this thesis has helped establishing such understanding.

Appendix A

Finite Dimensional Hilbertspaces

A *finite dimensional Hilbertspace* $\mathcal{H}$ is a complex vector space with an inproduct and norm, i.e. an ordered pair $(\mathcal{H}, K)$ where $\mathcal{H}$ is a set of elements, the *Hilbert-vectors* here denoted in Dirac notation as $|\,\alpha\rangle\,, |\,\psi\rangle\,, \ldots$ (called *kets*), and K is a field whose elements are termed scalars and are here restricted to the complex numbers $\mathbb{C}$. On $\mathcal{H}$ is defined an internal binary operation of *addition*, denoted by $+$, which is associative and commutative; Furthermore $\mathcal{H}$ is closed under linear combinations, i.e. *the superposition principle* holds:

$$a \in \mathbb{C},\ |\,\phi\rangle\,, |\,\psi\rangle \in \mathcal{H} \implies a\,|\,\phi\rangle \in \mathcal{H} \quad \text{and} \quad |\,\phi\rangle + |\,\psi\rangle \in \mathcal{H}. \tag{A.1}$$

There exists a distinguished element of $\mathcal{H}$, the *zero* vector, written *0* with the property that

$$\mathit{0} + |\,\phi\rangle = |\,\phi\rangle\,, \qquad \forall\,|\,\phi\rangle \in \mathcal{H} \tag{A.2}$$

which is proven to be unique. To every element of $\mathcal{H}$ there corresponds an *inverse* in the following sense

$$\forall\,|\,\phi\rangle \in \mathcal{H},\ \exists\,|\,\psi\rangle \quad \text{such that} \qquad |\,\phi\rangle + |\,\psi\rangle = \mathit{0}. \tag{A.3}$$

Furthermore, on $\mathcal{H}$ there is also defined an external binary operation of *scalar multiplication* which has the following properties. Let $a, b \in \mathbb{C},\ |\,\phi\rangle\,, |\,\psi\rangle \in \mathcal{H}$, then:

$$\begin{array}{ll} (a+b)(|\,\phi\rangle + |\,\psi\rangle) = a\,|\,\phi\rangle + a\,|\,\psi\rangle + b\,|\,\phi\rangle + b\,|\,\psi\rangle & \textit{distributive} \\ a(b\,|\,\phi\rangle) = (ab)\,|\,\phi\rangle & \textit{associative} \\ a\,|\,\phi\rangle \in \mathcal{H} & \\ 1\,|\,\phi\rangle = |\,\phi\rangle\,. & \end{array} \tag{A.4}$$

An *inner product* on $\mathcal{H}$ is a scalar-valued function defined on the Cartesian product $\mathcal{H} \times \mathcal{H}$, i.e. a function $f : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ where we write $f(|\,\phi\rangle\,, |\,\psi\rangle) = \langle\,|\,\phi\rangle|\,\psi\rangle$ with $|\,\phi\rangle$, $|\,\psi\rangle \in \mathcal{H}$. The inner product has the following properties:

$$\begin{array}{l} \langle\,\phi|\,\psi\rangle = \langle\,\phi|\,\psi\rangle^* \\ \langle\,\phi|\,a\psi\rangle = a\,\langle\,\phi|\,\psi\rangle \\ \langle\,\phi|\,(|\,\psi\rangle + |\,\chi\rangle) = \langle\,\phi|\,\psi\rangle + \langle\,\phi|\,\chi\rangle \\ \langle\,\phi|\,\phi\rangle \geq 0 \ \text{ and } \ \langle\,\phi|\,\phi\rangle = 0 \text{ iff } \ |\,\phi\rangle = \mathit{0}. \end{array} \tag{A.5}$$

Here * denotes complex conjugate, and $\langle\,\phi|$ is the adjoint vector of the corresponding ket $|\,\phi\rangle$. The function

$$\|\cdot\|:\mathcal{H}\to\mathbb{R},\quad \psi\mapsto\|\psi\|:=\sqrt{\langle\psi|\psi\rangle} \tag{A.6}$$

is referred to as the *norm* of $|\,\psi\rangle$.

A *complete orthonormal* set of *basis* vectors for $\mathcal{H}$ is a set of vectors $\{\alpha_1\ldots\alpha_i\}$ such that any $|\,\phi\rangle\in\mathcal{H}$ can be written in the form

$$|\,\psi\rangle=\sum_i^N c_i\,|\,\alpha_i\rangle \qquad c_i\in\mathbb{C}, \tag{A.7}$$

and the $|\,\alpha\rangle_i$ satisfy the orthonormality condition $\langle\,\alpha_i|\,\alpha_j\rangle=\delta_{ij}$ where δ_{ij} is the usual Kronecker delta symbol. The number N is the dimension of $\mathcal{H}$. From Eq.(A.7) the coefficients c_i are given by

$$c_i=\langle\,\alpha_i|\,\psi\rangle. \tag{A.8}$$

The completeness of the complete set of orthonormal vectors implies that

$$\sum_i^N=|\,\alpha_i\rangle\,\langle\,\alpha_i|=\mathbb{1}, \tag{A.9}$$

where $\mathbb{1}$ is the *identity operator*, i.e. $\mathbb{1}\,|\,\phi\rangle=|\,\phi\rangle$ for all $|\,\phi\rangle\in\mathcal{H}$.

This completes the definition of a *complex finite-dimensional Hilbertspace*: it is a finite dimensional complex vectorspace, with an inproduct related to the norm via Eq.(A.5).

Appendix B

Operators

A *linear and homogeneous* operator A on a Hilbert-space $\mathcal{H}$ is a *map* $A : \mathcal{H} \rightarrow \mathcal{H}$, $|\,\phi\rangle \longmapsto A\,|\,\phi\rangle$ such that

$$A(a\,|\,\phi\rangle + b\,|\,\psi\rangle) = aA\,|\,\phi\rangle + bA\,|\,\psi\rangle\,. \tag{B.1}$$

From Eq.(A.8) we see that for the vectors $|\,\psi\rangle \in \mathcal{H}$ a one-to-one correspondence exists with the set of complex numbers $\langle\,\alpha_i|\,\psi\rangle$. This allows us to represent the operator A as a $N \times N$ matrix A acting on the Hilbertspace $\mathbb{C}^N$ with matrixelements $\mathsf{A}_{ij} := \langle\,\alpha_i|\,A\,|\,\alpha_j\rangle$ and

$$A\,|\,\alpha_i\rangle = \sum_{i=1}^{N} \mathsf{A}_{ij}\,|\,\alpha_i\rangle\,. \tag{B.2}$$

The *adjoint* of a linear operator A is written $A^\dagger$ and defined by the relation

$$\langle\,\psi|\,A^\dagger\,|\,\phi\rangle = \langle\,\phi|\,A\,|\,\psi\rangle^*\,, \qquad \forall\,|\,\phi\rangle\,,|\,\psi\rangle \in \mathcal{H}. \tag{B.3}$$

Note that not all linear operators commute, i.e. for two linear operators A and B, their commutation $[A, B] := AB - BA$ is not necessarily zero. This is a property of operator-algebra which lies at the heart of quantum mechanics. An operator is *self-adjoint* if $A = A^\dagger$. An operator is *unitary* if $A^\dagger = A^{-1}$ where A^{-1} is the *inverse* of A. An operator is called *normal* if it commutes with its adjoint $[A, A^\dagger] = 0$. Furthermore an operator is called *hermitian* if it is true that

$$\langle\,\psi|\,A\,|\,\phi\rangle = \langle\,\phi|\,A\,|\,\psi\rangle^*\,, \qquad \forall\,|\,\phi\rangle\,,|\,\psi\rangle \in \mathcal{H}. \tag{B.4}$$

An operator is called *positive* iff $\langle\,\phi|\,A\,|\,\phi\rangle \geq 0$ for all $|\,\phi\rangle \in \mathcal{H}$, and is notated as $A \geq 0$. A *unitary* operator U preserves the inner product, i.e. $\langle\,U\psi|\,U\phi\rangle = \langle\,\psi|\,\phi\rangle$. Finally, an operator A on $\mathcal{H}$ is called *bounded* iff the set of positive numbers $\|A\,|\,\chi\rangle\,\|$ is bounded from above for $\|\,|\,\chi\rangle\,\| \leq 1$. The smallest upperbound is called the *norm* of A.

The *eigenvalues* of an operator A (dim $\mathcal{H} = N$) are the numbers α satisfying

$$A\,|\,\phi\rangle = \alpha\,|\,\phi\rangle\,, \qquad |\,\phi\rangle \neq \mathit{0}. \tag{B.5}$$

The vector $|\,\phi\rangle$ is then called the eigenvector belonging to the eigenvalue α. There can be at most N distinct eigenvectors. The set of all eigenvalues is called *the spectrum*. For A self-adjoint, it is proven that all the eigenvalues are real. It is then the case that it is always possible to choose a set $\{|\,\alpha_i\rangle\}$ of eigenvectors , $i = 1, 2 \ldots N$, which provide a complete orthonormal basis for A. The eigenvalue belonging to the eigenvector $|\,\alpha_i\rangle$ is denoted as α_i. Some of the α_i may be equal and then A is said to be *degenerate*. An eigenvalue α_i may be d_{α_i}-fold degenerate, in which case α_i generates a d_{α_i}-dimensional eigenspace: i.e. there are d_{α_i} orthogonal vectors $|\,\psi_{\alpha_i}\rangle$ which obey Eq.(B.5), thus forming a basis for a d_{α_i}-dimensional subspace of $\mathcal{H}$. For A non-degenerate, so that there are N distinct eigenvalues, the operator A is called *maximal*.

The *spectral theorem* in the finite-dimensional case is given (without proof) as:

Theorem B.0.1. *Every normal operator has a unique set of complete orthonormal, eigenvectors, the so called* eigenbasis *with the corresponding set of eigenvalues, and conversely every basis with eigenvalues determines uniquely a normal operator.(For proof see Ref. [46], page* 13.*)*

Appendix C

Projection Operators

The *direct sum* of two vector spaces is an operation denoted by '$\oplus$'. Consider the direct sum Hilbert space $\mathcal{H} = \mathcal{V} \oplus \mathcal{V}^{\perp}$. This is again a Hilbert space, and $\mathcal{V}$ and $\mathcal{V}^{\perp}$ are its respective orthogonal *subspaces*. Every vector $|\,\phi\rangle \in \mathcal{H}$ can be uniquely written as:

$$|\,\phi\rangle = \alpha\,|\,\phi\rangle_{\parallel} + \beta\,|\,\phi\rangle_{\perp}\,, \qquad |\,\phi\rangle_{\parallel} \in \mathcal{V},\ |\,\phi\rangle_{\perp} \in \mathcal{V}^{\perp}, \tag{C.1}$$

where $|\,\phi\rangle_{\parallel}$ and $|\,\phi\rangle_{\perp}$ are restricted to their respective subspaces and $|\alpha|^2+|\beta|^2 = 1$. The *projection operator* $P_{\mathcal{V}}$ onto $\mathcal{V}$ is defined by

$$P_{\mathcal{V}}\,|\,\phi\rangle := \alpha\,|\,\phi\rangle_{\parallel}\,. \tag{C.2}$$

In other words, $P_{\mathcal{V}}\,|\,\phi\rangle$ projects the state $|\,\phi\rangle$ onto the linear subspace $\mathcal{V}$. Then for the perpendicular vectors $|\,\phi\rangle_{\perp}$ it follows that $\beta\,|\,\phi\rangle_{\perp} = (\mathbb{1} - P_{\mathcal{V}})\,|\,\phi\rangle$. Projection operators are necessarily *idempotent* and *self-adjoint* linear operators, that is

$$P^2 = P = P^{\dagger}. \tag{C.3}$$

Projection operators have the following properties:

1. two projection operators P and Q are called orthogonal projections iff $PQ = 0$.
2. The sum of two orthogonal projection operators is again a projection operator;
3. The identity operator can be written in many ways as the sum of orthogonal projectors in $\mathcal{H}$;
4. The orthocomplement of a projection operator P is given by $P^{\perp} = \mathbb{1} - P$;
5. The eigenvalues of a projection operator are 0 and 1.

Going back to the subspaces $\mathcal{V}$ and $\mathcal{V}^{\perp}$ it then follows that $P_{\mathcal{V}} + P_{\mathcal{V}^{\perp}} = \mathbb{1}$, which means that every projection operator decomposes a Hilbertspace into a direct sum of two orthogonal subspaces. When viewed as measurement outcomes (see postulate 3, chapter 2.2) the eigenvalues of a projection operator indicate whether or not the state is in the subspace spanned by P.

Suppose that A is a maximal operator on $\mathcal{H}$ (dimension N) with eigenbasis $|\,\alpha_i\rangle$ and eigenvalues a_i. Let P_i be the projection operator onto the 1-dimensional subspace spanned by $|\,\alpha_i\rangle$. Then the following three relations hold:

$$P_i\,|\,\alpha_i\rangle = \delta_{ij}\,|\,\alpha_j\rangle\,, \quad \text{and} \quad P_iP_j = \delta_{ij}, \tag{C.4}$$

$$\sum_{i=1}^{N} P_i = \sum_{i=1}^{N} |\,\alpha_i\rangle\,\langle\,\alpha_i| = \mathbb{1}, \tag{C.5}$$

$$\sum_{i=1}^{N} a_iP_i = \sum_{i=1}^{N} a_i\,|\,\alpha_i\rangle\,\langle\,\alpha_i| = A. \tag{C.6}$$

Eq.(C.5) is referred to as the *resolution of the identity* or the *completeness relation* and Eq.(C.6) as the *spectral decomposition* of the operator A. In general, when the eigenvectors of an operator are not given by the basis $\{|\,\alpha_i\rangle\}$, A can be written as

$$A = \sum_{ij} a_{ij}\,|\,\alpha_i\rangle\,\langle\,\alpha_j|\,. \tag{C.7}$$

For A hermitian ($A^\dagger = A$), it follows that $a_{ij} = a^*_{ji}$.

Using the spectral decomposition of Eq.(C.6) we can define for a maximal operator A a complex function f on the spectrum of A as follows:

$$f(A) := \sum_{i=1}^{N} f(a_i)P_i. \tag{C.8}$$

This definition specifies the so-called *function of the operator* A itself.

We are now in the position to state the following important theorem:

Theorem C.0.2. *If two self adjoint operators A and B commute, then there exists a maximal self-adjoint operator C of which A and B are functions, i.e. $A = f(C)$ and $B = g(C)$; the converse follows for normal operators. (For proof see* Redhead, [46]*, page* 18.*)*

On the other hand, if $A = f(C)$ and the map f is not one-to-one, then there will always exist another maximal operator C' such that $A = g(C')$, and C and C' do not commute, i.e. $[C, C'] \neq 0$. They do commute iff A itself is maximal. In this case f can be inverted: $C = f^{-1}(A) = f^{-1}(g(A))$, from which it follows that $[C, C'] = 0$.

Note that if we can write $Q = f(S)$ for an observable Q as a function of some maximal observable S, then the choice of S is by no means unique .

Lastly, if two operators commute, it is always possible to find a basis relative to which these operators are simultaneously diagonal, and thus both operators then have all eigenvectors in common. However, if two operators do *not* commute, it does *not* follow that in every case they have no common eigenvectors, but only that all their eigenvectors are not common to both operators.

Appendix D

Tensor Product

The *tensor product of two vectors* $|\,\phi\rangle$ and $|\,\psi\rangle$ from Hilbertspaces $\mathcal{H}_1$ and $\mathcal{H}_2$ is written as $|\,\phi\rangle \otimes |\,\psi\rangle$ and satisfies the following relation

$$\Big(\sum_i a_i\,|\,\phi_i\rangle\Big) \otimes \Big(\sum_j b_j\,|\,\psi_j\rangle\Big) = \sum_{ij} a_i b_j\,|\,\phi_i\rangle \otimes |\,\psi_j\rangle \tag{D.1}$$

with $\forall\,|\,\phi_i\rangle \in \mathcal{H}_1, \forall\,|\,\psi_j\rangle \in |H_2 \quad \text{and} \quad \forall\ a_i, b_j \in \mathbb{C}$ The *tensor product of two Hilbertspaces* $\mathcal{H}_1$ and $\mathcal{H}_2$, written as $\mathcal{H}_1 \otimes \mathcal{H}_2$, is the set of all linear combinations of the tensor products of vectors selected from the two spaces. (More formally $\mathcal{H}_1 \otimes \mathcal{H}_2$ is the space of bilinear functionals defined over the Cartesian product of the dual spaces $\mathcal{H}_1'$ and $\mathcal{H}_2'$). $\mathcal{H}_1 \otimes \mathcal{H}_2$ is itself a vector space with a basis $\{|\,\alpha_i\rangle \otimes |\,\beta_j\rangle\}$ where $\{|\,\alpha_i\rangle\}$ is a basis for $\mathcal{H}_1$ and $\{|\,\beta_j\rangle\}$ is a basis for $\mathcal{H}_2$.

The *tensor product of two linear operators* A and B, where A acts on $\mathcal{H}_1$ and B acts on $\mathcal{H}_2$, is written as $A \otimes B$. It is iself a linear operator on $\mathcal{H}_1 \otimes \mathcal{H}_2$ and is defined by the relation

$$(A \otimes B)(|\,\phi\rangle \otimes |\,\psi\rangle) := A\,|\,\phi\rangle \otimes B\,|\,\psi\rangle\,, \quad \forall\,|\,\phi\rangle \in \mathcal{H}_1,\ \forall\,|\,\psi\rangle \in \mathcal{H}_1. \tag{D.2}$$

From this defintion it follows that $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$. As a special case of this result it follows that for self-adjoint operators A and B

$$f(A \otimes \mathbb{1}) \quad = f(A) \otimes \mathbb{1} \tag{D.3}$$

$$g(\mathbb{1} \otimes B) \quad = \mathbb{1} \otimes g(B). \tag{D.4}$$

It should be noted that *not* every operator on $\mathcal{H}_1 \otimes \mathcal{H}_2$ is of the form $A \otimes B$. The fact that this is not the case is of fundamental importance to the quantum state space. For notational brevity the tensor product symbol $\otimes$ is often omitted, yielding, e.g., $|\,\psi\rangle \otimes |\,\phi\rangle = |\,\psi\rangle\,|\,\phi\rangle$. Upon using this abbreviation notation one should always remember which state or operator is defined on which Hilbert space.

Finally we take a closer look at the vectors on the tensorproduct space. A general vector $|\,\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ can be written as

$$|\,\Psi\rangle = \sum_{j=1}^{N_1} \sum_{i=1}^{N_2} c_{jk}\,|\,\alpha_j\rangle \otimes |\,\beta_k\rangle\,, \tag{D.5}$$

where $c_{jk} = (\langle\,\alpha_j| \otimes \langle\,\beta_k|)\,|\,\Psi\rangle \in \mathbb{C}$ and N_1, N_2 are the dimensions of respectively $\mathcal{H}_1$ and $\mathcal{H}_2$.

However, the direct product vector $|\,\phi_1\rangle \otimes |\,\phi_2\rangle$ written in the corresponding basis reads:

$$\sum_{j=1}^{N_1} a_j\,|\,\alpha_j\rangle \otimes \sum_{k=1}^{N_2} b_k\,|\,\beta_k\rangle = \sum_{j=1}^{N_1}\sum_{k=1}^{N_2} a_j b_k\,|\,\alpha_j\rangle \otimes |\,\beta_k\rangle\,. \tag{D.6}$$

Eq.(D.6) is a special case of Eq.(D.5), namely the case where $c_{jk} = a_j b_k$. The special vectors which can be written as in Eq.(D.6), that is in the form $|\,\phi_1\rangle \otimes |\,\phi_2\rangle$, are called *direct-product-vectors* or *separable*. Vectors which can not be written in this form are called *non-separable* or *entangled*.

Lastly, we state the so-called *Schmidt or bi-orthogonal decomposition* for bipartite systems. For every vector $|\,\Psi\rangle$ in $\mathcal{H}_1 \otimes \mathcal{H}_2$ there exist two *orthonormal bases* $\{|\,\bar{\phi}_i\rangle\}$ in $\mathcal{H}_1$ and $\{|\,\bar{\psi}_i\rangle\}$ in $\mathcal{H}_2$ such that $|\,\Psi\rangle$ can be written in the form

$$|\,\Psi\rangle = \sum_i d_i\,|\,\bar{\phi}_i\rangle \otimes |\,\bar{\psi}_i\rangle\,, \tag{D.7}$$

where by convention $d_i \geq 0$. This family of positive numbers $\{d_i\}$ is called the family of *Schmidt-coefficients*. To get this Schmidt-representation, the bases of the subsystems in Eq.(D.6) and Eq. (D.7) are transformed into each other by a unitary transformation:

$$|\,\bar{\phi}_i\rangle_1 = \sum_k U_{ik}\,|\,\alpha_k\rangle_1 \quad \text{and} \quad |\,\bar{\psi}_j\rangle_2 = \sum_l U_{jl}\,|\,\beta_l\rangle_2\ . \tag{D.8}$$

The Schmidt decomposition is unique (up to phasefactors) iff the d_i are non-degenerate. If the dimension of the Hilbertspace of the two subsystems are N_1 and N_2 respectively, the sum in Eq. (D.7) runs up to the dimension of the smallest Hilbert space.

Lastly, the following two features of the Schmidt decompostion are important:

1. The Schmidt decomposition allows us to give a different criterium than the one just mentioned for a state $|\,\Psi\rangle$ in $\mathcal{H}_1 \otimes \mathcal{H}_2$ to be entangled, namely iff the number of non-zero Schmidt-coefficients is greater than one.

2. There is no Schmidt decomposition theorem for a system with more than two subsystems.

Appendix E

Maps and Partial Transposition

In this appendix a summary will be given of background knowledge about states, operators and maps in quantum mechanics. Using this knowledge is essential for understanding of the so-called partial transpose criterion for the separability of (bi-partite) density operators. This appendix is a reformulation of work in Ref. [51].

Single Systems

Consider the physical system described by a set of states $\{|\psi_i\rangle\}$. The linearity and superposition principle of quantum mechanics imply that this set spans a Hilbert space $\mathcal{H}$ of dimension d, which is a complex vector space with an orthonormal basis.

A set of higher objects can now be defined on $\mathcal{H}$, i.e. we consider the set of *linear* operators $\{A_k\}$ whose elements transform one state to another:

$$A : |\phi\rangle \longrightarrow |\psi'\rangle\,. \tag{E.1}$$

The set of all linear operators $\{A_k\}$ in turn define a Hilbert space $\mathcal{H}\otimes\mathcal{H}$ of dimension d^2 when a suitable inner product is chosen. One of such an inner product is $< A, B >= \mathrm{Tr}[A^* B]$.

An even higher set of objects called *maps* can now be defined and is denoted by $\{\mathcal{M}\}$. Its elements linearly transform the set of operators into itself:

$$\mathcal{M} : A \longrightarrow A' = \mathcal{M}(A) \tag{E.2}$$

These maps are so called *super-operators* that act on the Hilbertspace $\mathcal{H}\otimes\mathcal{H}$. An example of such a map is the unitary transformation $U : A \rightarrow A' = U^\dagger A U$. The set of all maps constitutes a Hilbertspace $\mathcal{H}^{\otimes 4}$ of dimension d^4. Using the concept of non-negative operators we now define *positive* maps.

Definition E.0.1. *A map $\mathcal{M}$ is positive if for every non-negative operator A the operator $A' = \mathcal{M}(A)$ is again a non-negative operator.*

The map $\mathcal{M}$ is *trace-preserving* when $Tr[A'] = Tr[A]$ for every A. Trace-preserving positive maps are of special importance, since they transform the set of density operators to itself. This property may lead one to expect that these maps correspond to physical processes or symmetries. However, in quantum mechanics *not all* positive trace-preserving maps can be associated with physical processes [51]. As we will see in the next section, this fact becomes relevant when considering composite systems.

Composite Systems

Consider two systems A and B with respective states $\{\,|\,\phi_i\rangle^A\}$ and $\{|\,\psi_j\rangle^B\}$ on $\mathcal{H}^A$ and $\mathcal{H}^B$ with dimension d_A and d_B. The states of the composite system can be written on the tensorproduct states $|\,\phi_i\rangle^A \otimes |\,\psi_j\rangle^B$ generating $\mathcal{H}^A \otimes \mathcal{H}^B$ of dimension $d_A \times d_B$. Similarly, the set of linear operators $\{A_j\}$ on $\mathcal{H}^A \otimes \mathcal{H}^B$ generates a Hilbertspace of dimension $(d_A \times d_B)^2$, and the set of maps generates a Hilbertspace of dimension $(d_A \times d_B)^4$. Suppose we have a map $\mathcal{M}_A$ on subsystem A. When this map is positive and trace-preserving it transforms density operators to density operators. When system A is part of a composite system $A{+}B$ we ask when a positive map of system A, leaving system B unchanged, would transform a density operator defined on the composite system again into a density operator. That is, we ask when the *extended* map $\mathcal{M}_{AB} = \mathcal{M}_A \otimes \mathbb{1}_B$ is again positive?

Definition E.0.2. *A map $\mathcal{M}_A$ is called* c*ompletely positive if all its extensions are positive.*

An interesting fact is that there exist maps which are positive, but not completely positive. An important case of such a map is the transpose. To see this, consider for example the singlet state $|\,\Psi\rangle = \frac{1}{\sqrt{2}}(|\,0\rangle\,|\,1\rangle - |\,1\rangle\,|\,0\rangle)$ of a two-level bi-partite system. The transpose T of this state for the first system is simply the exchange of the bra's and ket's in the density matrix for this particular single system. This is a positive map. However, the extended transpose, or the *partial* transpose[1], on the composite system $PT = T_A \otimes \mathbb{1}_B$ is not positive, as can be easily seen by noting the negative eigenvalues of the partial transpose. Thus T, although positive, is not completely positive.

The fact that positive but not completely positive maps on a subsystem do not necessarily transform density operators on the composite system to density operators, can be exploited to detect or witness entanglement. This is the key to the partial transpose criterion which is the topic of the next section.

Partial Transpose Criterium

To answer the question if a given composite system, characterised by a density operator ρ is separable or not, one needs necessary and sufficient criteria. One of such necessary criteria is the Peres-Horodecki partial transpose criterion [61, 62]. Recall that a density operator ρ of two systems $A + B$ is separable iff it can be written as

$$\rho = \sum_i p_i \rho_i^{(A)} \otimes \rho_i^{(B)}, \tag{E.3}$$

[1]The partial transpose O^{T_A} of an operator O on $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ is defined in terms of is matrix elements with respect to a given basis by $\langle\, k, l|\, O\,|\, m, n\rangle = \langle\, m, l|\, O^{T_A}\,|\, k, n\rangle$. Note that ρ^{T_A} is basis-dependent but its spectrum is not.

with $p_k > 0$ and $\sum_i p_i = 1$. Now consider the transpose of an operator A:

$$T : A \longrightarrow A^T. \tag{E.4}$$

As shown above this is a trace-preserving positive, but not completely positive map. Thus the extension to the *partial transpose* $PT = T_A \otimes \mathbb{1}_B$ is not positive on the composite system. Under the partial transpose PT, the separable density operator of Eq.E.3) transforms as follows:

$$PT : \rho \longrightarrow \rho' = \sum_i p_i \left(\rho_i^{(A)}\right)^T \otimes \rho_i^{(B)}. \tag{E.5}$$

As $(\rho^{T_A})^{T_B} = \rho^T$ and because $\rho^T \geq 0$ always holds, positivity of ρ^{T_A} implies positivity of ρ^{T_B}. Now recall that because T is positive $\left(\rho_i^{(A)}\right)^T$ is again a density operator. Therefore ρ' is again a density operator. We now look at the eigenvalues of ρ'. If ρ is seperable then ρ' has positive eigenvalues. Therefore, if ρ' has one or more negative eigenvalues, the original density operator ρ must have been non-seperable, i.e. entangled. This is the *partial transpose criterium.* For a general density operator it is only a necessary condition for separability .

However, for Hilbertspaces $\mathcal{H}_2 \otimes \mathcal{H}_2$ and $\mathcal{H}_2 \otimes \mathcal{H}_3$ the partial transpose criterium is both necessary and sufficient [62] for separability. That is, ρ is separable iff the eigenvalues of its partial transpose ρ' are positive (then ρ is said to be a *PPT state*). For higher dimensional Hilbertspaces this is no longer the case. It is known that there exist density operators which are not seperable (i.e entangled), but for which the eigenvalues of ρ' are non-negative. Such states are said to exhibit *bound* entanglement [59]. The general opinion is that these states can not be distilled or purified. (See chapter 3.3).

Whether or not there also exist sufficient criteria for separability using the partial transpose for states of more than two systems (three or N-partite systems) is still under investigation [59].

Appendix F

Classical vs. Quantum mechanical State Space

In this appendix I will show three radical differences between the classical and quantum mechanical formalisms: the difference in the respective (i) state spaces, (ii) observables and (iii) probability theories.

Let me first briefly summarize the classical state space and the observables defined on this space. In the classical context, to a given physical system one associates a measurable space Ω, the so-called *phase space*, which carries information about the different degrees of freedom of the physical system. The states are classically represented as probability measures on Ω; among them are the measures concentrated at a point of Ω, which correspond to maximal information about the preparation of the system and are called the *pure states*. The set of physical properties determine the position of the system in the phase space Ω; and conversely the physical properties of the system can be directly determined from the coordinates of the point in phase space. Thus, a *one-to-one correspondence* exists between systems and their physical properties and the mathematical representation in terms of points in phase space. Mixed systems or ensembles are described by *mixed states* which are *unique* convex combinations of the extremal elements, the pure states. *Observables* in classical physics are described as real valued functions on Ω, so that a pure state (a point of Ω) determines a well defined value of each observable at all times of the evolution of the system. This is in accordance to the requirements of determinism, i.e. at all times the physical state uniquely determines the measurable properties of the system.

In quantum mechanics the state space and observables are represented quite differently. The states which are represented by vectors in Hilbertspace are not determined in the same way as in classical physics by measurable properties of an individual system. In general, a quantum state does not correspond uniquely to the outcomes of the measurements that can be performed on the system. This can be seen as follows. In appendix C, we have seen that the state pure state P_ψ assigns a probability distribution to an orthogonal set of states (one of them being $|\psi\rangle$) which is completely concentrated onto the vector $|\psi\rangle$. P_ψ can thus be regarded as the analogon of δ-distribution on the classical phase space Ω. However the radical difference is that the one-dimensional projection operators do not (in general) form an *orthonormal* set. This implies that the pure state P_ψ

will also assign a positive probability to P_ϕ if $\langle \phi | \psi \rangle \neq 0$. This is contrary to the classical case, where the pure state $\delta(q - q_0, p - p_0)$ concentrated on $(p_0, q_0) \in \Omega$ will always assigns a probability zero to *every other* pure state. Furthermore, the probability that the value of an observable B lies in the real interval X when the system is in the state ρ is $Tr\,(\rho P_{B,X})$ where $P_{B,X}$ is the projector associated to the pair (B, X) by the spectral theorem for self-adjoint operators. One could say that this outlines 'quantum indeterminism'[49] since $Tr\,(\rho P_{B,X})$ is in general not concentrated in $\{0, 1\}$ even when ρ is a pure state.

Apart from these differences in the state space and the observables defined on them, the third difference between the classical and quantum mechanical formalism is that the relation of QM with probability theory is nonclassical. In the standard classical formalism of probability theory probabilities are assigned to events which, in classical physics, can be defined in terms of subsets of a state space. In classical mechanics, for example, one generally works with probability distributions that are measures on a collection of subsets of the phase space [75]. The probabilities $p(A_i)$ computed in QM, however are probabilities not assigned to subsets A_i but to *subspaces* $\mathcal{A}_i$ of the Hilbert space, and the standard additivity requirement

$$\sum_i p(A_i) = p\Big(\bigcup_i A_i\Big) \qquad \text{for disjoint } A_i \tag{F.1}$$

is replaced by

$$\sum_i p(\mathcal{A}_i) = p\big(\otimes_i \mathcal{A}_i\big) \qquad \text{for orthogonal } \mathcal{A}_i \tag{F.2}$$

Accordingly, the standard formalism of QM requires modifications to probability theory.

The above mentioned differences can also be recognized when realizing that for both QM and classical mechanics every mixed state admits a convex decomposition in terms of pure states, and that this decompostion is unique in the classical case while it is *never* unique in the quantum case. Furthermore, any quantum mechanical pure state can be transformed *continuously* and reversibly along a path through the pure states to any other pure state, whereas this is not necessarily the case for classical pure states.[1] In other words, it is not the Hilbertspace itself that is the fundamental and characteristic feature of quantum mechanics, but rather the specific way the Hilbertspaces are divided up into into factorspaces that marks the divergence of the classical formalism [82]. It is this special way of dividing up into factorspaces that allows for the typical non-classical features of superpositions and entanglement.

[1] Hardy [50] sees this as the fundamental distinction in his axiomatic formulation of quantum mechanics

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Abbreviations

LR	local realism
HV	hidden variables
QM	quantum mechanics
CQM	completeness of quantum mechanics
EPR	Einstein-Podolsky-Rosen
EPRB	Einstein-Podolsky-Rosen-Bohm
LOCC	local operations and classical communication
CLOCC	collective local operations and classical communication
SLOCC	stochastic local operations and classical communication
PLHV	partial local hidden variable theory
CHSH	Clauser-Horne-Shimony-Holt
BI	Bell-inequality
BK	Bell-Klyshko inequality
SI	Svetlichny inequality
GHZ	Greenberger-Horne-Zeilinger
PPT	positive partial transpose
NPPT	non-positive partial transpose
NPT	non-positive partial transpose
PVM	projection valued measure
POVM	positive operator valued measure
CSCO	complete set of commuting observables