universität wien

MASTERARBEIT

Titel der Masterarbeit

„Higher order interference theories. Assessing a class of extensions to quantum mechanics.“

Verfasser

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angestrebter akademischer Grad

Master of Science (MSc)

Wien, 2013

Studienkennzahl lt. Studienblatt:	A 066 876
Studienrichtung lt. Studienblatt:	Masterstudium Physik
Betreuerin / Betreuer:	Ao. Univ.-Prof. Mag. Dr. Časlav Brukner

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1. Introduction

The aim of this thesis is to examine certain theories that are more general than quantum mechanics. Quantum mechanics itself can be understood to describe interference of order 2, as described by density matrices. Here we consider those generalizations of quantum mechanics that allow for higher order interference terms. The motivation for this assessment was given by the *density cube theory*, developed by Dakić, Paterek and Brukner [13], which accounts for interference of third order. I will show that the density cube theory, as well as any other higher order interference theory which adds interference of order n (and only n) to quantum interference cannot achieve the following two natural requirements for a generalization of quantum mechanics: (1) recovering quantum mechanics as a special case and (2) predicting experimental results differing from it.

In chapter 2 I will give a short review of conditions, in form of inequalities, which are imposed on classical mechanics. These spatial and temporal inequalities, allowing to experimentally discriminate between classical and quantum physics, will be presented for different cases, as well as the maximal bound attainable in quantum theory.

In chapter 3 I will present a summary of the theory of density cubes (following Ref. [13]), which allows for third-order interference. It is shown that only for systems with three or more degrees of freedom the density cube theory is different from ordinary quantum mechanics. A transformation T for density cubes is then introduced, which allows to violate the quantum bound for temporal inequalities.

Chapter 4 contains a novel analysis of the theory of density cubes and similar higher order interference theories. First, it will be shown that the transformation T for density cubes is (considering that composite systems are obtained using the tensor product) not completely positive, and hence not physically realisable. Then the general theorem of incompatibility between higher order interference theories of arbitrary order n and quantum mechanics will be proven: no theory adding the possibility for interference of order n (and only n) can both satisfy conditions (1) and (2) from above. Finally, the connection between density cube theory and the strength of signalling is discussed, and a modification of T is presented ($\hat{T}$), which allows maximal violation of the quantum bound.

2. Inequalities in classical and quantum mechanics

In this chapter, we will review some some basic facts about the foundations of quantum mechanics. After a brief recapitulation of elementary quantum theory, we will give a summary of spatial and temporal inequalities which allow to discriminate classical from quantum theories and derive bounds imposed on quantum theory itself, allowing differentiation from other, "more non-classical" theories.

2.1. Summary of quantum mechanics

This section will serve as a reminder of standard quantum mechanics (of a closed system), as it will be used in the subsequent developments. We will rely on a concise modern formulation, using texts by Sakurai [32], Shankar [34], Peres [28], Nielsen and Chuang [24] as well as Paris [26].

2.1.1. State vector formalism

We consider a Hilbert space $\mathscr{H}$. Physical states in quantum theory are represented by vectors $|\psi\rangle$ ("kets", following Dirac's terminology) in the Hilbert space: $|\psi\rangle \in \mathscr{H}$.[1] Every linear combination of state vectors again leads to a valid ket:

$$|\psi\rangle = \alpha\,|\psi_1\rangle + \beta\,|\psi_2\rangle\,, \tag{2.1}$$

where α and β are complex numbers – this is known as *the superposition principle*.

The *dual space* $\mathscr{H}^*$ contains the dual vectors ("bras"), obtained through a one-to-one *dual correspondence*: $|\psi\rangle \overset{DC}{\leftrightarrow} \langle\psi|$. Addition of bra vectors again yields a bra vector. The dual to $\alpha\,|\psi\rangle$ is $\alpha^*\,\langle\psi|$; note the complex conjugation of the multiplicative term.

We can define an *inner product* between bra and ket vectors $\langle\cdot|\cdot\rangle : \mathscr{H}^* \times \mathscr{H} \to \mathbb{C}$, which has conjugate symmetry, is sesquilinear and positive definite:

$$\boxed{\begin{aligned} \langle\psi_1|\psi_2\rangle &= \langle\psi_2|\psi_1\rangle^* \\ \langle\alpha\psi_1|\beta\psi_2\rangle &= \alpha^*\beta\,\langle\psi_1|\psi_2\rangle \\ \langle\psi|\psi\rangle &\geq 0, \quad \forall\,|\psi\rangle\,. \end{aligned}} \tag{2.2}$$

Further require all state vectors $|\psi\rangle$ representing physical states to be normalized, meaning that $\langle\psi|\psi\rangle = 1$; we will soon see why.

Composite systems We can consider states of composed systems as states on a Hilbert space of higher dimension, which is the tensor product of the Hilbert spaces describing the components of the system. Consider $\mathscr{H}_1$ describing some degree of freedom and $\mathscr{H}_2$ describing another one. Then to describe a system having both degrees of freedom, we will recur to a state vector $|\psi\rangle \in \mathscr{H}_1 \otimes \mathscr{H}_2$. This can be repeated any number of times.

Note that, while some composite states $|\psi\rangle \in \mathscr{H}_1 \otimes \mathscr{H}_2$ can be expressed as tensor products of states $|\psi_1\rangle \in \mathscr{H}_1$ and $|\psi_2\rangle \in \mathscr{H}_2$, some cannot, like:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle \otimes |\psi_2\rangle + |\psi_1'\rangle \otimes |\psi_2'\rangle). \tag{2.3}$$

We thus distinguish between the former, *product states* and the latter, *correlated* (or "entangled") states, which have very peculiar properties, to which we will come in section 2.2.

[1] Note the difference with classical mechanics, where physical states are represented by their position $\mathbf{x}$ and momentum $\mathbf{p}$ at each time. We will see the connection of a state in the Hibert space to position and momentum in section 2.1.3.

Transformations What does it mean to transform a state vector $|\psi\rangle \mapsto |\psi'\rangle$? The resulting ket has to be normalized, and the transformation linear because of the possibility of superposition in quantum theory.

Operators U leaving the inner product invariant are *unitary operators*, meaning $U^\dagger U = UU^\dagger = \mathbf{1}$. It is always possible to write the physical evolution of a closed quantum system as a unitary transformation: $|\psi'\rangle = U|\psi\rangle$. We will see in section 2.1.3 how to specify the evolution of a system in the Hamiltonian and Lagrangian picture.

Measurements Let us turn to the concept of measurement, which is very different from the one in classical mechanics. In the quantum formalism, each measurable observable X is associated to a *measurement operator*, acting on a ket and resulting in another ket: $|\psi\rangle \mapsto X(|\psi\rangle)$.

Measurement operators X are hermitian, therefore, their eigenvalues X_i are real and their eigenvectors $|X_i\rangle$ form an orthogonal base spanning the whole Hilbert space. We can write them as a sum of projectors:

$$\boxed{X = \sum_i X_i |X_i\rangle\langle X_i|,} \tag{2.4}$$

where $\sum_i |X_i\rangle\langle X_i| = \mathbf{1}$ (completeness relation) holds.

Now when a state is measured, the outcome will be X_i with the probability[2] $|\langle\psi|X_i\rangle|^2$. After the measurement, the state will be "projected" into one of the eigenstates $|X_i\rangle$, corresponding to the result P_i which was obtained in the measurement process.

We can define the *expectation value* of a measurement operator with respect to a state $|\psi\rangle$ as

$$\langle A\rangle = \langle\psi|A(\psi)\rangle = \sum_i X_i |\langle\psi|X_i\rangle|^2 \tag{2.5}$$

One can ask if, making one first measurement X_1 then X_2 is the same as first measuring X_2 and then X_1. The answer is no, the two results will only be the same if the operators A and B are *compatible*, meaning they commute ($[A,B] = AB - BA = 0$), which is only the case if they share the same eigenbase.

A final word about a more generalized picture of measurements. One can also consider *non-projective* measurements. The measurement operator then can be expressed as a sum of $X = \sum_i X_i M_i^\dagger M_i$, where the required condition $\sum_i M_i^\dagger M_i = \mathbf{1}$, which can be fulfilled even if the X_i are not projectors. This type of measurement is known as *P(ositive) O(perator)-V(alued) M(easure)*. It is interesting that a POVM measurement can always be translated to a projective measurements of a composite system of which the original system is a part.

2.1.2. Statistical mixtures

The formalism described until now does not take into account *statistical mixtures* of different states. Suppose we prepare particles in a state ψ_1 and other ones in a state ψ_2; now if we consider the entire ensemble of prepared particles, this does not correspond to a coherent superposition $1/\sqrt{2}(\psi_1 + \psi_2)$ (which would mean all particles had the same state after all), but rather to a statistical mixture; such mixture is also present in classical mechanics.

To take this kind of operation into account, we define a state ρ as the sum of the projectors corresponding to the mixed states $|\psi_k\rangle$, multiplied with their relative frequency p_k:

$$\boxed{\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|,} \tag{2.6}$$

[2] This is *Born's rule*, which explains why we required $\langle\psi|\psi\rangle = 1$ earlier, as this corresponds to the sum of the probabilities for all outcomes.

where $\sum_k p_k = 1$, meaning that $\mathrm{Tr}[\rho] = 1$. It can readily be shown that ρ also is positive and hermitian. If we do not mix different states, then ρ is simply a projector. In the more general case, $\mathrm{Tr}[\rho^2] \leq 1$, the lower the trace of ρ^2 is, the higher the degree of mixture.

The density matrices are linear operators in $L(\mathcal{H})$, which is a Hilbert space of its own – the inner product between ρ_1 and ρ_2 is thus:

$$(\rho_1, \rho_2) = \mathrm{Tr}[\rho_1 \rho_2] \tag{2.7}$$

It is important that different mixtures may result in the same density operator, meaning they cannot be physically distinguished.

Composite systems Composite systems are to be treated by simple extension of the state vector formalism: consider $|\psi\rangle = 1/\sqrt{2}(|\psi_1\rangle \otimes |\psi_2\rangle + |\psi_1'\rangle \otimes |\psi_2'\rangle)$ then the corresponding (pure) density matrix is $\rho = |\psi\rangle\langle\psi|$, which can be written out as

$$\begin{aligned}\rho &= \frac{1}{2}(|\psi_1\rangle\langle\psi_1| \otimes |\psi_2\rangle\langle\psi_2| + |\psi_1'\rangle\langle\psi_1'| \otimes |\psi_2'\rangle\langle\psi_2'| + |\psi_1'\rangle\langle\psi_1'| \otimes |\psi_2\rangle\langle\psi_2|) + |\psi_1\rangle\langle\psi_1| \otimes |\psi_2'\rangle\langle\psi_2'| \\ &\neq \frac{1}{2}(|\psi_1\rangle\langle\psi_1| \otimes |\psi_2\rangle\langle\psi_2| + |\psi_1'\rangle\langle\psi_1'| \otimes |\psi_2'\rangle\langle\psi_2'|),\end{aligned} \tag{2.8}$$

the second line (without off-diagonal elements) would express a *mixed* state, while the first one is pure.

In density matrix formalism, we may also go from a composite to a constituent system, ignoring some degrees of freedom of the original density operator ρ_{AB}, and only considering a subsystem ρ_A. The corresponding operation is the *partial trace*:

$$\boxed{\rho_A = \mathrm{Tr}_B[\rho_{AB}] = \sum_i \langle i_B|\rho_{AB}|i_B\rangle\,,} \tag{2.9}$$

where $|i_B\rangle$ form a base for the subsystem B. The resulting ρ_A is a valid (positive, trace 1) density operator. Note that the same reduced density matrix can be obtained by partial trace of different density matrices.

Measurements Measurement operators can be applied to density matrices through natural generalization of (2.5). In essence, the expectation value with respect to ρ becomes:

$$\langle A\rangle = \mathrm{Tr}[\rho A]. \tag{2.10}$$

General quantum maps General quantum operations in the density operator picture are operators $M(\rho) : L(\mathcal{H}) \to L(\mathcal{H})$, meaning $M \in L(L(\mathcal{H}))$, which itself is a Hilbert space. It has to be noted that such operators include unitary transformations ($M(\rho) = U\rho U^\dagger$) but also other types of transformations, like mixing ($M(\rho) = \alpha(\rho) + (1-\alpha)\rho'$) which are not accessible in the vector formalism.

Physically relevant maps are (1) linear, (2) trace-preserving and (3) positive, meaning they map density operators to density operators. An even stronger requirement, in the light of composite systems is *complete positivity*, meaning that the tensor product of identity operator (for a Hilbert space of arbitrary dimension) and the map: $\mathbf{1} \otimes M$ has to be positive.

In conclusion, physically meaningful quantum maps have to be trace-preserving, linear and completely positive; they do not reduce to unitary transformations.

2.1.3. Dynamics

To conclude the section about elementary quantum theory, we will investigate what the dynamics of the state vector (or the density operator) look like. We will start with the Lagrangian formulation and then look at the (more widely applicable) Hamiltonian formalism.

Lagrangian approach – Feynman path integrals The first formulation of dynamics is the Feynman path integral one. It stems from the intuition that, for a particle in quantum mechanics different paths can contribute to a transition amplitude, whereas in the classical case (loosely, when $\hbar \to 0$) only one path is taken. In this formulation, the standard classical action $S = \int L_{\text{classical}}(x, \dot{x})\mathrm{d}t$ is used to calculate the propagators between two small time steps:

$$\langle x_n, t_n | x_{n-1}, t_{n-1} \rangle = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \exp\left(\frac{i\int_{t_{n-1}}^{t_n} L_{\text{classical}}\mathrm{d}t}{\hbar}\right), \tag{2.11}$$

which can be repeatedly applied, so as to get the propagator for a finite time step:

$$\langle x_N, t_N | x_0, t_0 \rangle = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{N/2} \int \mathrm{d}x_{N-1} \int \mathrm{d}x_{N-2} \cdots \int \mathrm{d}x_1 \prod_{n=1}^{N} \exp\left(\frac{i\int_{t_{n-1}}^{t_n} L_{\text{classical}}\mathrm{d}t}{\hbar}\right), \tag{2.12}$$

which is *Feynman's path integral*. The computation of these integrals is often very cumbersome and thus the alternative Hamiltonian formulation is preferred; fundamentally both are equivalent, and we can derive Schrödinger's equation from the propagator of an infinitesimal time step.

Hamiltonian approach – Schrödinger equation The idea in the Hamiltonian approach is to start from infinitesimal time evolution operators $U(t_0+\mathrm{d}t, t_0) = 1 - i\Omega\mathrm{d}t$. The generator Ω of the time evolution, has the dimension of frequency. The Hamiltonian H, which in classical mechanics corresponds to the generator of time evolution, is naturally connected to Ω through $\Omega = H/\hbar$, thus we can write $U(t+\mathrm{d}t, t_0) = 1 - iH\mathrm{d}t/\hbar$. From there, and exploiting the property of composition:

$$U(t_2, t_1) = U(t_2, t_1)U(t_1, t_0), \tag{2.13}$$

we can derive Schrödinger's equation for time evolution operator:

$$U(t+\mathrm{d}t, t_0) - U(t, t_0) = -\frac{iH}{\hbar}\mathrm{d}tU(t, t_0) \tag{2.14}$$

$$i\hbar\frac{\partial}{\partial t}U(t, t_0) = HU(t, t_0). \tag{2.15}$$

Now, we just have to multiply operators in (2.15) with the state kets to obtain Schrödinger's equation for state vectors:

$$\boxed{i\hbar\partial_t |\psi\rangle = H|\psi\rangle\,.} \tag{2.16}$$

In the density matrix formalism, we can easily derive an analogous equation from (2.16) and (2.6):

$$\boxed{i\hbar\partial_t\rho = -[\rho, H],} \tag{2.17}$$

which has the same form as Liouville's theorem in statistical mechanics, the commutator taking the place of the Poisson bracket.

2.2. Spatial inequalities

In this section, we will examine ways to distinguish quantum from classical behaviour experimentally, using spatially separated measurements. First, a two-observer, two-setting, two-outcome setup will be examined and then generalizations to an arbitrary number of observers and of measurement settings will be presented.

2.2.1. Bell and CHSH formulation

The possibility of an *experimentum crucis*, allowing to test the validity of the quantum picture against a hidden variable model (which was supposed to make a *complete theory* out of quantum mechanics), was first theoretically proposed by J. S. Bell in 1964 [7].

Bell's setup The setup of the initial thought experiment is the following: there are two observers Alice and Bob, each being able to measure some arbitrary dichotomic observable, independently of each other. We send each observer a system, which he/she measures using an an arbitrary measurement setting (we will think of a "spin particle" and therefore a measurement setting will correspond to a spatial direction along which the spin will be measured). We repeat this procedure, to obtain correlations between the results of both observers.

Suppose we can supplement hidden variables λ to the state vector $|\psi\rangle$, so that the outcomes (A for Alice and B for Bob) are to be predicted fully by λ and the choice of the observable by the experimentalist (denoted by $\mathbf{a}$ and $\mathbf{b}$ respectively). This is what is generally called *realism*:

$$A(\mathbf{a},\mathbf{b},\lambda) = \pm 1, \quad B(\mathbf{a},\mathbf{b},\lambda) = \pm 1, \tag{2.18}$$

the second requirement is that the choice of Alice ($\mathbf{a}$) does not influence Bob's outcome and vice-versa. We call this *locality*. Together with realism (2.18), we obtain *local realism*

$$\boxed{A(\mathbf{a},\lambda) = \pm 1, \quad B(\mathbf{b},\lambda) = \pm 1.} \tag{2.19}$$

Using this condition, we can obtain the experimental expectation value of the product of A and B (the correlator) by integrating over the (normalized) probability distribution of the hidden variables $p(\lambda)$:

$$E(\mathbf{a},\mathbf{b}) = \int \mathrm{d}\lambda\, p(\lambda) A(\mathbf{a},\lambda) B(\mathbf{b},\lambda), \tag{2.20}$$

now Bell derived an inequality from (2.20) and (2.19):

$$\boxed{|E(\mathbf{a},\mathbf{b}) - E(\mathbf{a},\mathbf{c})| \leq 1 + |E(\mathbf{b},\mathbf{c})|,} \tag{2.21}$$

which can be violated by the quantum singlet state $|\psi\rangle = 1/\sqrt{2}(|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle)$, where $|\pm\rangle$ are the

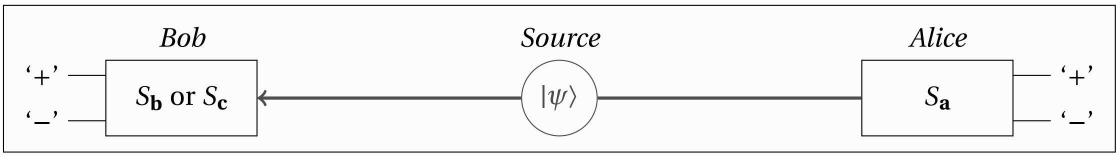


Figure 2.1: *Bell setup: A source produces an entangled the entangled two-particle state $|\psi\rangle$. One particle is sent to Alice, one to Bob. Alice measures the spin $S_{\mathbf{a}} = \mathbf{S}\cdot\mathbf{a}$ on her side and Bob measures either $S_{\mathbf{b}} = \mathbf{S}\cdot\mathbf{b}$ or $S_{\mathbf{c}} = \mathbf{S}\cdot\mathbf{c}$ on his side.*

eigenkets of the spin operator S_z, and where the spin is measured in arbitrary directions (e.g. $S_{\mathbf{a}} = \mathbf{S}\cdot\mathbf{a}$). Consider the case $\mathbf{a}\cdot\mathbf{c} = 0$ and $\mathbf{b}\cdot\mathbf{c} = \mathbf{a}\cdot\mathbf{b} = 1/\sqrt{2}$ then the quantum version of (2.21) is:

$$|\langle S_{\mathbf{a}} \otimes S_{\mathbf{b}}\rangle - \langle S_{\mathbf{a}} \otimes S_{\mathbf{c}}\rangle| - |\langle S_{\mathbf{b}} \otimes S_{\mathbf{c}}\rangle| = \sqrt{2} - 1 > 1, \quad \text{(quantum)} \tag{2.22}$$

which violates the local realist bound of (2.21). However, this inequality cannot be used for an experimental test.[3]

[3]It can be derived from the CHSH form, using the assumption that one expectation value is exactly 1, which is never empirically realised.

CHSH form Bell found that there could be a way to tell local realistic hidden variable theories from standard quantum mechanis, using a relatively simple thought experiment. A simpler, more symmetric and experimentally viable derivation, using two possible measurement directions on each side, was proposed by Clauser, Horne, Shimony and Holt in 1969 [11]. The derived "CHSH"-inequality has become the standard one for two-level systems with two spatially separated observers, and was used for the first conclusive experiment falsifying the local realistic hidden variable theory [2].

We will use a further simplified derivation of CHSH, given by Clauser and Horne in 1974 [10]. Again, consider only dichotomic observables (whose outcomes are either $+1$ or -1), and several runs of the experiment. Each observer now has two possible measurement directions ($\mathbf{a}$ and $\mathbf{a}'$ for Alice and $\mathbf{b}$ and $\mathbf{b}'$ for Bob), of which each observer can choose freely for each run.

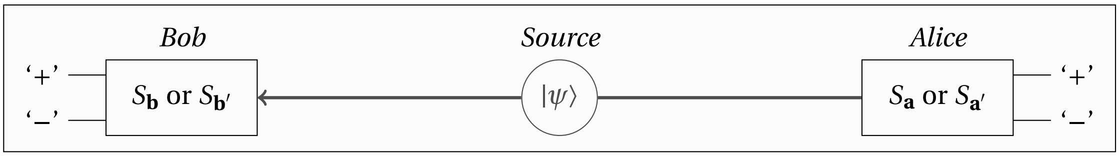


Figure 2.2: *CHSH setup: A source produces an entangled the entangled two-particle state $|\psi\rangle$. One particle is sent to Alice, one to Bob. Alice measures the spin $S_\mathbf{a} = \mathbf{S}\cdot\mathbf{a}$ or $S_{\mathbf{a}'} = \mathbf{S}\cdot\mathbf{a}'$ on her side and Bob measures either $S_\mathbf{b} = \mathbf{S}\cdot\mathbf{b}$ or $S_{\mathbf{b}'} = \mathbf{S}\cdot\mathbf{b}'$ on his side.*

Now consider local hidden variables, which supposedly determine the outcome (A, A' for Alice's two directions and B, B' for Bob's) of any measurement direction, then the following equation holds (for any *single* run):

$$A(B+B') + A'(B-B') = \pm 2, \tag{2.23}$$

because $A, A', B, B' = \pm 1$, and each outcome is fully determined by the hidden variables before it is measured (realism). If we take the expectation of (2.23) over many runs, we get the CHSH inequality for the correlators:

$$\boxed{|E(\mathbf{a},\mathbf{b}) + E(\mathbf{a},\mathbf{b}')| + |E(\mathbf{a}',\mathbf{b}) - E(\mathbf{a}',\mathbf{b}')| \leq 2.} \tag{2.24}$$

This inequality can again be violated by the singlet state and spin-measurements $S_\mathbf{a} = \mathbf{S}\cdot\mathbf{a}$, $S_{\mathbf{a}'} = \mathbf{S}\cdot\mathbf{a}'$ on Alice's side and $S_\mathbf{b} = \mathbf{S}\cdot\mathbf{b}$ and $S_{\mathbf{b}'} = \mathbf{S}\cdot\mathbf{b}'$ on Bob's, using directions such that $\mathbf{a}\cdot\mathbf{a}' = \mathbf{b}\cdot\mathbf{b}' = 0$ and $\mathbf{a}\cdot\mathbf{b} = \mathbf{a}\cdot\mathbf{b}' = \mathbf{a}'\cdot\mathbf{b} = -\mathbf{a}'\cdot\mathbf{b}' = 1/\sqrt{2}$ so that:

$$|\langle S_\mathbf{a}\otimes S_\mathbf{b}\rangle + \langle S_\mathbf{a}\otimes S_{\mathbf{b}'}\rangle| + |\langle S_{\mathbf{a}'}\otimes S_\mathbf{b}\rangle - \langle S_{\mathbf{a}'}\otimes S_{\mathbf{b}'}\rangle| = 2\sqrt{2} > 2 \quad \text{(quantum)}. \tag{2.25}$$

2.2.2. Generalization to more observers

Different inequalities, using dichotomic observables and based on local realistic hidden variable theories were proposed over time.

Mermin's inequalities One category is due to Mermin [23]. For n observers, we define the *Mermin operator* M_n:

$$M_n = \frac{1}{2i}\left(\bigotimes_{j=1}^{n}(S_x^j + iS_y^j) - \bigotimes_{j=1}^{n}(S_x^j - iS_y^j)\right), \tag{2.26}$$

which leads to the sum of all permutations, where there is an odd number of S_x in the correlator, i.e.

$$\begin{aligned} M_n = & S_y^1\otimes S_x^2\otimes S_x^3\otimes\cdots\otimes S_x^n + S_x^1\otimes S_y^2\otimes S_x^3\otimes S_x^n \\ & + S_y^1\otimes S_y^2\otimes S_y^3\otimes S_x^4\otimes\cdots\otimes S_x^n + \ldots \\ & + S_y^1\otimes S_y^2\otimes S_y^3\otimes S_y^4\otimes S_y^5\otimes S_x^6\otimes\cdots\otimes S_x^n + \ldots \\ & + \ldots, \end{aligned} \tag{2.27}$$

where each line stands for all permutations of the uneven number of S_y. Mermin showed that using local realistic hidden variables, the bound for the expectation value of M_n was:

$$\boxed{\begin{aligned} E(M_n) &\leq 2^{n/2} \quad (n \text{ even}) \\ E(M_n) &\leq 2^{(n-1)/2} \quad (n \text{ odd}), \end{aligned}} \tag{2.28}$$

whereas for the so-called "GHZ-state" (named after Greenberger, Horne and Zeilinger [16], who discovered their relevance for four particles and observers) $\psi_{GHZ} = 1/\sqrt{2}(|+\rangle \otimes |+\rangle \cdots \otimes |+\rangle + i(|-\rangle \otimes |-\rangle \cdots \otimes |-\rangle))$, the expectation value can reach:

$$\langle M_n \rangle = \langle \psi_{GHZ} | M_n | \psi_{GHZ} \rangle = 2^{n-1}. \tag{2.29}$$

Incidentally, this shows that while there is a violation of the inequality for both even and odd n, for an odd n, the violation is larger, which (at least theoretically) does not recur to the statistical nature used in the Bell and CHSH arguments above [16].

Belinskii-Klyshko-inequalities While Mermin's inequality does not include the CHSH one as a special case, Belinskii and Klyshko [6] derived a generalization of them to more observers, which also includes Mermin's inequalities (for uneven N)

Using the two-observer inequality as a starting point, the definition of the measurement operators S_N inequalities is recursive:

$$\begin{aligned} S_N &= \frac{1}{2} S_{N-1} \otimes (A_N + (-1)^N A'_N) + (-1)^{[N/2]} \frac{1}{2} S'_{N-1} \otimes (A_N + (-1)^{N+1} A'_N) \\ S'_N &= \frac{1}{2} S'_{N-1} \otimes (A'_N + (-1)^N A_N) + (-1)^{[N/2]} \frac{1}{2} S_{N-1} \otimes (A'_N + (-1)^{N+1} A_N) \\ S_0 &= S'_0 = 1 \end{aligned} \tag{2.30}$$

where A_N and A'_N are the operators for the N-th observer and $[N/2]$ means the non-integer part of the division is discarded. It can be shown that the local realistic bound for the expectation value of S_N is bounded by ± 1:

$$|E(S_N)| \leq 1, \tag{2.31}$$

whereas in the quantum case, with respect to the n-particle GHZ-state, we can obtain:

$$\langle S_N \rangle = \langle \psi_{GHZ} | S_N | \psi_{GHZ} \rangle = 2^{(n-1)/2}, \tag{2.32}$$

which is also the amount of the violation of the inequality (incidentally, this is the same as for the Mermin-inequalities).

Werner-Wolf-Zukowski-Brukner-inequalities The most general description of local realistic inequalities for multiple observers and dichotomic observables was given by Werner and Wolf [39], and independently by Zukowski and Brukner [40]. We follow here Zukowski and Brukner, who use a procedure similar to the one used in the 1974 derivation of the CHSH inequality [10]: start with the outcomes of *two* measurements per observer – for each observer i, $A_1^{(i)} = \pm 1$ and $A_2^{(i)} = \pm 1$. Then the following algebraic identity holds, provided we consider a local realistic hidden variable theory:

$$\sum_{s_1,\ldots,s_N=\pm 1} S(s_1,\ldots,s_N) \prod_{i=1}^{N} (A_1^{(i)} + s_i A_2^{(i)}) = \pm 2^N, \tag{2.33}$$

provided that $S(s_i) = \pm 1$. Then, taking the expectation value as a statistical outcome, the bound follows

$$\left| \sum_{s_1,\dots,s_N=\pm 1} S(s_1,\dots,s_N) \sum_{k_1,\dots,k_N=1,2} s_1^{k_1-1} s_2^{k_2-1} \cdots s_N^{k_N-1} E(k_1,\dots,k_N) \right| \leq 2^N. \tag{2.34}$$

These 2^{2^N} different inequalities for different choices of the sign function $S(s_1,\dots,s_N)$ can be reduced to 2^N. Because for $|\dots+1(\dots)+\dots|$ and for $|\dots-1(\dots)+\dots|$ (i.e. changing just one sign in the sum) the inequality has to hold, we have expressions of the type $|a+b| \leq 2^N$ and $|a-b| \leq 2^N$ thus $|a|+|b| \leq 2^N$. We can repeat this for each particular term in the sum, thus:

$$\boxed{\sum_{s_1,\dots,s_N=\pm 1} \left| \sum_{k_1,\dots,k_N=1,2} s_1^{k_1-1} s_2^{k_2-1} \cdots s_N^{k_N-1} E(k_1,\dots,k_N) \right| \leq 2^N.} \tag{2.35}$$

It can be shown that this characterization is *complete*, meaning each set of correlators obeying (2.35) can be described by a local realistic theory. This formulation therefore is the most general possible for two-outcome observable local realistic theories.

2.2.3. Generalization to non-dichotomic observables

Another type of generalization of the standard CHSH scenario is to take observables with more than two outputs into account. Some specific work on three-state systems ("qutrits") was done; an inequality was constructed [19] and it was shown that they can violate local realism stronger than qubits [9]. For quNits, for $N \leq 16$ numerical work showed that the quantum states violating local realism become more and more resistant to mixing with noise [14].

Finally, Collins et al. [12] derived a *general* local realistic inequality for arbitrarily high dimensional systems. The formulation becomes more complicated than in the dichotomic case.

Consider Alice and Bob, still with two measurement setups from which they can freely chose, but this time, their measurement outcomes A_1, A_2, B_1, B_2 can take N values. We will call $P(A_1 = B_1)$ the probability that both outcomes are the same, $P(A_1 = B_1 + 1)$ that the outcome of A is the outcome of B plus one (modulo N), and so on. For $N = 3$, a simple inequality follows from applying the usual condition of local realism:

$$\begin{aligned} &[P(A_1 = B_1) + P(B_1 = A_2 + 1) + P(A_2 = B_2) + P(B_2 = A_1)] \\ -&[P(A_1 = B_1 - 1) + P(B_1 = A_2) + P(A_2 = B_2 - 1) + P(B_2 = A_1 - 1)] \leq 2, \end{aligned} \tag{2.36}$$

which can be generalized to arbitrary N:

$$\boxed{\begin{aligned} \sum_{k=0}^{[N/2]-1} \left(1 - \frac{2k}{N-1}\right) &([P(A_1 = B_1 + k) + P(B_1 = A_2 + k + 1) + P(A_2 = B_2 + k) + P(B_2 = A_1 + k)] \\ &-[P(A_1 = B_1 - k - 1) + P(B_1 = A_2 - k) + P(A_2 = B_2 - k - 1) + P(B_2 = A_1 - k - 1)]) \leq 2. \end{aligned}} \tag{2.37}$$

This can be violated by $\phi = \frac{1}{\sqrt{N}} \sum_j^N |j\rangle_A \otimes |j\rangle_B$.[4] The amount of violation depends on N, and as $N \to \infty$, the sum of (2.37) goes to ≈ 2.698. Note that the experimental realization of non-dichotomic observables is challenging, as a setup to discriminate between several different outcomes is more complex than one differentiating between only two outcomes.

[4]Interestingly, an even *stronger* violation occurs for non-maximally entangled states (of the same form but with weights different from $1/\sqrt{N}$), as shown by Acin et al. [1].

2.3. Temporal inequalities

The superposition principle (with complex phases, see (2.1)) is at the origin of the discrepancy between local realist hidden variable theories and quantum theories. The fact that superposition is not spatially restricted, but can be upheld for composite systems leads to the violation of Bell type inequalities.

2.3.1. Formulation

Can quantum behaviour be distinguished from classical behaviour by looking at their temporal evolution? It turns out that it can, if we translate classical behaviour as *macroscopic realism* together with *noninvasive measurability at macroscopic level*; Leggett and Garg first proposed an inequality on temporal correlations derived from these conditions [22].

Macroscopic realism means that a macroscopic system will at all times be in a definite state and noninvasive measurement (at macroelevel) means that measurements do not disturb the (macroscopic) state. [5] We consider a single observer, making different measurements on the same system, over time. The outcomes are $A_i = \pm 1$, where i is a temporal index.

In this formalism, the two conditions are equivalent to the existence of a joint probability distribution $p(A_1, A_2 \dots A_n)$ where the normalization condition reads

$$\sum_{A_i=\pm 1} p(A_1, A_2, \dots, A_n) = 1, \tag{2.38}$$

and we can obtain any probability for specific outcome(s) by summing over the irrelevant outcomes. The simplest inequality that can be obtained from this uses three different times at which measurements are conducted and is derived like this:

$$\begin{aligned} &E(A_1,A_2)+E(A_2,A_3)+E(A_1,A_3)+1 = P_{12}(++)+P_{12}(--)-P_{12}(+-)-P_{12}(-+)\\ &+P_{23}(++)+P_{23}(--)-P_{23}(+-)-P_{23}(-+)+P_{13}(++)+P_{13}(--)-P_{13}(+-)-P_{13}(-+)+1\\ &=3P(+++)+3P(---)-P(+--)-P(-+-)-P(--+)-P(++-)-P(-++)+1\\ &=4P(+++)+4P(---)\geq 0, \end{aligned} \tag{2.39}$$

interestingly, its form reminds one of the initial Bell-inequality (2.21). One can also easily derive all Leggett-Garg inequalities of the CHSH-form, with four time steps:

$$\boxed{|E(A_1,A_2)+E(A_2,A_3)|+|E(A_1,A_4)-E(A_2,A_4)| \leq 2} \tag{2.40}$$

Generalizations to even more temporal measurements have been given [4, 5], but we will not go into detail as the concept is simple.

2.3.2. Violation by quantum mechanics

We have not yet discussed if and how Leggett-Garg-type inequalities are violated by quantum systems. Interestingly, it turns out that *every* quantum state (micro- or macroscopic) undergoing time-evolution (see section 2.1.3 for a reference) stemming from a non-trivial Hamiltonian violate them, provided the measurement accuracy is high enough [21]. It is only when the accuracy is reduced that

[5] The notion of "state" is different in macrorealism and quantum mechanics. One can readily reject the requirement of non-invasiveness for quantum mechanics, as we have seen that measurements always alter the quantum system in section 2.1.1. Even if the quantum state is changed, this does not necessarily imply that the macrostate has to change. Furthermore, one can devise *negative measurements*, where the measurement operator interacts with the system only if it is in a certain state, otherwise not.

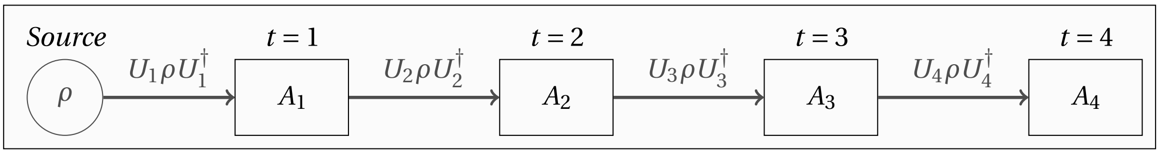


Figure 2.3: *Leggett-Garg setup with four consecutive dichotomic (negative) measurements A_1 to A_4. For each run, only* two *measurements are made (e.g. at $t=1$ and $t=4$ or at $t=2$ and $t=3$), at the other times the state is left alone. Between the measurements the state undergoes unitary evolution.*

macrorealism is respected [20]. This is in stark contrast with the spatial picture, where only certain (microscopic) quantum states are potentially violating the local realistic picture.

Experimental violation of Leggett-Garg-inequalities was achieved only recently [3, 18, 25], thus proving the assumptions of macrorealism and non-invasive measurement to be inadequate.

2.4. Relation between spatial and temporal inequalities

Considering the surprising similarity of Bell- and Leggett-Garg-type inequalities, one might ask if there is a deeper equivalence between both formulations. The first answer is that there is not, at least on the classical side of the formulation: macrorealism and non-invasiveness are not equivalent to local realism. However, on the quantum mechanical side, both types of correlations may somehow be connected or can potentially reduced to one another. Specially when assessing non-quantum transformations (as we will do in section 3.3), the question will be of particular interest (see section 4.2.4). For now let us concentrate on general considerations.

2.4.1. Temporal correlators

The first step needed to make sense of the relation between spatial and temporal inequalities is to study the quantum counterpart to the correlations $E(A_i, A_j)$.

From Fritz [15], we know that for two operators A and B the temporal correlator $\langle AB\rangle$ is given by half the anticommutator:

$$\langle AB\rangle = \frac{1}{2}\langle\psi|\{A,B\}|\psi\rangle\,, \tag{2.41}$$

as the anticommutator is symmetric, it follows that it does not depend on which measurement was carried out first.

We can readily extend this to correlators between three measurements:

$$\langle A_1 A_2 A_3\rangle = \frac{1}{4}\langle\psi|\{\{A_1, A_2\}, A_3\}|\psi\rangle\,, \tag{2.42}$$

which generalizes by repeated application to:

$$\langle A_1 \ldots A_n\rangle = \frac{1}{2^{n-1}}\langle\psi|\{\{\{\ldots\{\{A_1, A_2\}, A_3\}\ldots\}, A_{n-1}\}, A_n\}|\psi\rangle\,. \tag{2.43}$$

One can thus permute each measurement with all the measurements made before, without affecting the single correlator.

2.4.2. The Tsirelson Bound

One feature that both the usual spatial CHSH inequality (2.24) and the Leggett-Garg inequality with four time steps (2.40) share is the limitation imposed by quantum mechanics. Unlike for Mermin's inequalities (2.28), for which with an appropriate quantum state, the *logical bound* of the inequality can be saturated (meaning the sum of all correlators equals the number of correlators), in this case, it can't.[6]

An enlightening explanation of the quantum bound $2\sqrt{2}$ for the spatial CHSH inequality was derived by Tsirelson [37, 38]. He showed that the following two statements are (among others) equivalent:

- There exist Hilbert spaces $\mathscr{H}_1$ (dimension m) and $\mathscr{H}_2$ (dimension n) with hermitian operators A_k and B_l on $\mathscr{H}_1$ and $\mathscr{H}_2$ respectively, which all square to $\mathbb{1}$ and a density matrix $\rho \in L(\mathscr{H}_1 \otimes \mathscr{H}_2)$. Then the correlator matrix C_{kl} is given by $C_{kl} = \mathrm{Tr}[\rho(A_k \otimes B_l)]$
- In Euclidean space of dimension $\min(m, n)$ there exist vectors $\mathbf{x_k}$ and $\mathbf{y_l}$, with $|\mathbf{x_k}| \leq 1$ and $|\mathbf{y_l}| \leq 1$ so that the correlator matrix C_{kl} is given by $C_{kl} = \mathbf{x_k} \cdot \mathbf{y_l}$.

from the second formulation the bound of $2\sqrt{2}$ is simple to derive: one simply has to rotate four unity vectors in a plane and maximize the expression $\mathbf{x_1} \cdot \mathbf{y_1} + \mathbf{x_1} \cdot \mathbf{y_2} + \mathbf{x_2} \cdot \mathbf{y_1} - \mathbf{x_2} \cdot \mathbf{y_2}$ (see figure 2.4).

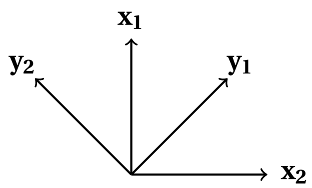


Figure 2.4: *Choice of vectors to saturate Tsirelson's bound for the CHSH-inequality*

Interestingly, Tsirelson's proof was extended to temporal correlations, Fritz [15] showing that the two statements given above are also equivalent to

- There exists a Hilbert space $\mathscr{H}$ with hermitian operators A_i and B_l on $\mathscr{H}$, which all square to $\mathbb{1}$, and a density matrix $\rho \in L(\mathscr{H})$. Then the correlator matrix C_{kl} is given by: $C_{kl} = \mathrm{Tr}[\rho \frac{1}{2}\{A_k, B_l\}]$, where $\{,\}$ is the anticommutator.

The $\Rightarrow$ direction is proven by taking $A_k \otimes \mathbb{1}$ as new A_k, and $\mathbb{1} \otimes B_k$ as new B_k. The $\Leftarrow$ direction works the same as Tsirelson's original proof. [37].

So it is clear that both in the spatial CHSH inequality (2.24) and the Leggett-Garg inequality with four time steps (2.40) share the same bound, $2\sqrt{2}$, attainable in quantum mechanics.

2.4.3. Generalization to more measurements

It is relatively simple to extend Tsirelson's proof to spatial or temporal correlators with more terms, of the form $\langle A_1 \dots A_n \rangle$. We will sketch the idea for the (non-normalized) Belinskii-Klyshko inequalities of even order (for the odd orders we already know that the quantum bound can saturate the logical bound).

The strategy is to take the correlator $\langle A_1 \dots A_n \rangle$, where the A_i are dichotomic observables, squaring to $\mathbb{1}$, as a simple two-observable correlator. Thus we will define $\mathscr{A}_1 := A_1 \otimes A_2 \otimes \cdots \otimes A_{n/2-1}$ and $\mathscr{A}_2 := A_{n/2} \otimes \cdots \otimes A_n$ (for the spatial case, in the temporal case, the concept is the same, we would use the anticorrelator formulation (2.43)), whence $\langle A_1 \dots A_n \rangle = \langle \mathscr{A}_1 \mathscr{A}_2 \rangle$.

Now we know from Tsirelson that we can associate to $\mathscr{A}_1$ and $\mathscr{A}_2$ a unit vector in the plane, and calculate the correlations as vector products between those vectors. Consider the inequality (local realistic scenario) obtained from (2.30) for four-correlators (remember for the i-th observer we have two

[6] In the spatial case, the concept of *PR-boxes* (named after Popescu and Rohrlich [29]) shows that it is possible to imagine stronger than quantum correlations, while still no information transfer between Alice and Bob is involved, and where the logical bound of the CHSH inequality is saturated.

possible settings, leading to the outcomes A_i and A'_i), where e.g. $4A^3A'$ means all four permutations of one A' and three A:

$$S_4 = |A^4 + 4A^3A' - 6A^2A'^2 - 4AA'^3 + A'^4| \leq 4. \tag{2.44}$$

now if we group the operators we have $A_1 \otimes A_2$, $A_1 \otimes A'_2$, $A'_1 \otimes A_2$ and $A'_1 \otimes A'_2$ for the first two and $A_3 \otimes A_4$, $A_3 \otimes A'_4$, $A'_3 \otimes A_4$ and $A'_3 \otimes A'_4$ for the last two. Out of these we can construct all four-correlators. We represent them as vectors in the plane, and try to maximize the violation of (2.44). After a relatively lengthy derivation, one obtains the optimal configuration seen in figure 2.5, obtaining $8\sqrt{2}$ as maximal value for $\langle S_4 \rangle$.

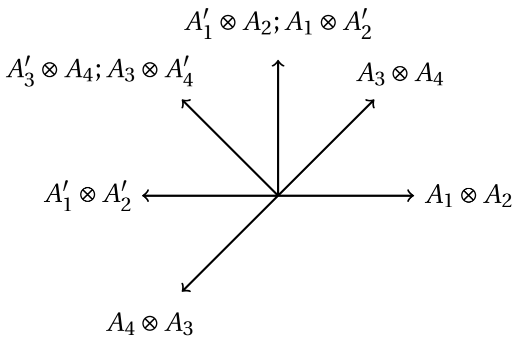


Figure 2.5: *Vectors saturating the generalized Tsirelson bound for the 4-dimensional Belinskii-Klyshko inequality* (2.44).

Generalizing this concept to arbitrarily high n yields the following optimal configuration given in figure 2.6, where the operators for the first half of the correlator have associated angles $0, \pi/2, \pi, 3\pi/2$ (in red) and for the other half $\pi/4, 3\pi/4, 5\pi/4, 7\pi/4$ (in blue). We will not prove this is the optimal

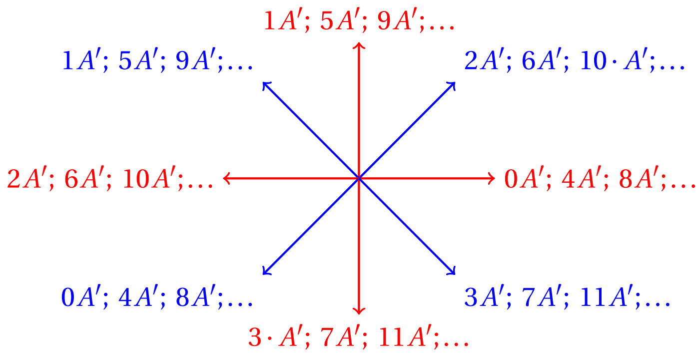


Figure 2.6: *Generalized Tsirelson bound for n-dimensional Belinskii-Klyshko inequalities. In red the vectors for the first $n/2$ operators, in blue the other ones. By $1A'$; $5A'$; $9A'$ we understand that permutations including either one, five, nine A'.*

configuration, however it yields the known bound of $2^{N-1}\sqrt{2}$ and provides a nice geometrical generalization of the known standard CHSH case (figure 2.4).

2.4.4. A general translation?

The fact that for both spatial and temporal correlator inequalities, the quantum bound can be derived the same way gives a further indication that a general translation from one direction to the other might actually be achievable, uncovering a deeper symmetry in quantum theory.

The Choi-Jamiolkowski-isomorphism [17] allows us to express a complete positive quantum map as a density operator on a higer dimension Hilbert space. We use the isomorphy between density operators $\rho_P \in L(\mathcal{H} \otimes \mathcal{H})$ and linear "superoperators" $P : L(\mathcal{H} \otimes \mathcal{H}) \to L(\mathcal{H} \otimes \mathcal{H})$. The isomorphy between P and ρ_P is given as follows:

$$\boxed{\rho_P = (\mathbb{1} \otimes P)\,|\phi^+\rangle\langle\phi^+|,} \tag{2.45}$$

where $|\phi^+\rangle = \sum_i^n |i\rangle \otimes |i\rangle$, when $\dim \mathcal{H} = n$. Now look at the correlator $\langle A \otimes B\rangle$ for the state $\rho = \rho_P$:

$$\langle AB\rangle = \mathrm{tr}[\rho_P(A \otimes B)] \tag{2.46}$$

$$= \mathrm{tr}[|\phi^+\rangle\langle\phi^+|(A \otimes P^*(B)] \tag{2.47}$$

$$\overset{\text{part. tr}}{=} \frac{1}{n}\mathrm{tr}[AP^*(B)], \tag{2.48}$$

Considering $P(\rho)$ is a temporal evolution: $P(\rho) = U(t_0, t)\rho U^\dagger(t_0, t)$. Using the Heisenberg picture[7] and setting $B = A_{t_0}$, then $\frac{1}{n}\mathrm{tr}[A_{t_0} P^*(A_{t_0})]$ represents the correlator in Heisenberg picture $\langle A_{t_0} A_{t_1}\rangle$ for the fully mixed state $\rho_M = \frac{1}{n}\mathbb{1}_n$ (where $\mathbb{1}_n$ denotes the unity of dimension n).

This means that it is possible to translate every spatial correlation on any Hilbert space $\mathcal{H} \otimes \mathcal{H}$ into a temporal one on the space $\mathcal{H}$, where the transformation is the same but the initial state is the fully mixed state $\mathbb{1}_n / n$.

The other way around, translating every temporal correlation into a spatial one does not work, except for ρ_M, the fully mixed state.[8] Therefore, from Choi-Jamiolkowski, the Tsirelson bound for the spatial scenario follows from the one derived in the temporal case, but not the other way around.

It may well be possible to achieve such a transformation using a different approach. Fritz supposedly proves a strong equivalence (i.e. in both directions) in his paper. Unfortunately, it is only an equivalence between spatial correlations on $\mathcal{H} \otimes \mathcal{H}$ and "temporal" correlations *on the very same space*. Basically, it states that Alice and Bob can perform their measurements after each other without changing the correlations (which is clear anyway because Alice's and Bob's operators commute). Or, said in another way, Fritz uses the trivial fact that [15, Prop. 2.1]:

$$A \otimes B = \frac{1}{2}\{A \otimes \mathbb{1}, \mathbb{1} \otimes B\}, \tag{2.49}$$

which is of no help for finding a deeper link between spatial and temporal scenarios.

[7] Basically, this means that we consider the state remains invariant, and the operators X evolve under Schrödinger's equation, using the equation $i\hbar\partial_t X = [X, H]$, which bears close resemblance to (2.17).

[8] This comes from the fact that any other state than ρ_M carries information and would allow for signalling in the CHSH scenario.

3. Violating the temporal quantum bound – density cubes

In this chapter, we will discuss the theory of *density cubes* (we follow the discussion by Dakić, Paterek and Brukner [13]), which provides an extension of quantum mechanics to take account of potential interference of third order. After introducing the concept in the first and second sections, we will present a transformation for a certain class of density cubes, which allows for some non-quantum behaviour. In the last section, we will show how this behaviour can violate the temporal Tsirelson bound for a Leggett-Garg type inequality, opening the way to an experimental test of the theory against standard quantum mechanics.

3.1. Third-order interference

In this section, we will examine the meaning of *third-order* interference, as implied in the density cube theory, which will be exposed in the next section. First, a brief summary of *second-order* interference will be given, to show what it can and can't amount to. Afterwards we will consider the quantum measure theoretic formulation of quantum mechanics, which generalizes naturally to higher order interferences. Finally, three interpretations of third-order interference in the standard quantum framework will be described.

3.1.1. *Second-order* interference

Intuitively, the special feature of *superposition*, appearing in quantum mechanics (see section 2.1), accounts for interference. We can have a state in the superposition of arbitrarily many base states: $|\psi\rangle = \sum_i c_i |i\rangle$, as long as $\sum_i |c_i|^2 = 1$. From this representation, it is not clear why there is a limitation to *second-order* interference. Rather, one would think that each of the base kets can be interfering with all others.

The density matrix formalism is best suited to show why there can be no higher order interference. The density operator corresponding to ψ would be $\rho = \sum_{ij} |i\rangle\langle j| c_i c_j^*$. The matrix entry $\rho_{ij} = c_i c_j^*$ represents the interference term between $|i\rangle$ and $|j\rangle$, and the density matrix is fully filled by such entries, it has no place for higher order terms.

3.1.2. Quantum measure theory and generalizations to higher order interference

Quantum measure theory [35, 36] originates in the idea that the wavefunction is not a good ontological base for the quantum theory. It is possible to describe quantum behavior without it (and without its mysterious "collapse") by allowing quantum probabilities to originate from a measure that does not obey Kolmogorov's sum rule for probabilities P of disjoint sets A and B:

$$P(A \sqcup B) - P(A) - P(B) = 0, \tag{3.1}$$

which simply states that the probability for either A or B is the sum of the probabilities for A and B respectively, if A and B are disjoint sets.

If we want to define a quantum measure μ, it will have to take into account second-order interference I_2

$$I_2(A,B) = \mu(A \sqcup B) - \mu(A) - \mu(B) \neq 0, \tag{3.2}$$

whereas the third order interference I_3 is still forbidden:

$$I_3(A,B,C) = \mu(A \sqcup B \sqcup B) - \mu(A \sqcup B) - \mu(B \sqcup C) - \mu(A \sqcup C) + \mu(A) + \mu(B) + \mu(C) = 0. \tag{3.3}$$

Following Sorkin, we can easily define arbitrarily high order interference terms

$$I_n(A_1, A_2, A_3, \dots A_n) = \mu(A_1 \sqcup A_2 \sqcup \dots \sqcup A_n) - \sum_{\text{perm.}} I_{n-1} + \sum_{\text{perm.}} I_{n-2} - \sum_{\text{perm.}} I_{n-3} \dots, \tag{3.4}$$

where $\sum_{\text{perm.}}$ denotes summing over all permutations. An theory is said to be of n-th order if $I_{n+1} = 0$, and therefore quantum theory is of the second order, and density cube theory of the third order.[9]

3.2. Density cubes

In standard quantum theory, as reviewed in section 2.1, the state is represented by a density operator $\rho \in L(\mathcal{H})$; it has trace 1 and is positive. This operator can be represented as a *matrix* ρ_{ij} with respect to a given basis $|i\rangle$:

$$\rho = \sum_{ij} \rho_{ij} |i\rangle \langle j| . \tag{3.5}$$

The fact that the density operator only has two indices accounts for the fact that quantum theory can only give an account of second order interference (ρ_{ij} represents this interference between the states $|i\rangle$ and $|j\rangle$, therefore there are not enough degrees of freedom in the density operator to give a description of three-state interference (see section 3.1.1 for more details).

An intuitive way to generalize to higher order interferences, taking the matrix form of ρ as a starting point, is to simply add more indices. In Ref. [13] this approach has been taken, making a "density cube" ρ_{ijk} out of a density matrix.

In analogy with the usual density matrix, we require the density cube to have trace one and to be positive:

$$\boxed{\sum_i \rho_{iii} = 1, \quad \rho_{iii} \geq 0 \quad \forall i} \tag{3.6}$$

Furthermore, we can generalize the scalar product to the density cube case:

$$\boxed{(\sigma, \rho) = \sum_{ijk} \rho^*_{ijk} \sigma_{ijk},} \tag{3.7}$$

still requiring that (σ, ρ) is a real number (so as to be able to use the probability interpretation of the scalar product), this can be achieved if, for cyclic permutations ($\pi(\cdot)$), we get the same entry and for anticyclic permutations ($\pi[\cdot]$), the complex conjugate:

$$\rho_{ijk} = \rho_{\pi(ijk)} = \rho_{\pi[ijk]}, \tag{3.8}$$

which is the analogue to the hermiticity condition for usual quantum density operators. When ρ is a pure state, we also expect $(\rho, \rho) = 1$.

3.2.1. The qubit case

First, we investigate a two-level system. The normalization and hermiticity conditions then are:

$$\rho_{112} = \rho^*_{122} = \rho^*_{121} = \rho_{211} \tag{3.9}$$
$$\rho_{122} = \rho^*_{112} = \rho^*_{212} = \rho_{221} \tag{3.10}$$
$$\rho_{111} \geq 0, \quad \rho_{222} \geq 0 \tag{3.11}$$
$$\rho_{111} + \rho_{222} = 1, \tag{3.12}$$

whence, we have three real degrees of freedom, for example ρ_{111}, ρ_{112} and ρ_{122}. Let us set $\rho_{112} = x_1/\sqrt{6}$, $\rho_{122} = x_2/\sqrt{6}$ and $\rho_{111} = (1 + x_3)/2$. The $x_1^2 + x_2^2 + x_3^2 = 1$, which means the pure states can be

[9] ρ_{123} in density cube is equivalent to $I_3(1,2,3)$ in this formalism.

identified to usual qubit states on the Bloch sphere. Hence we can define the "Pauli cubes":

$$\sigma_0 = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right\} \tag{3.13}$$

$$\sigma_1 = \sqrt{\frac{2}{3}} \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \right\} \tag{3.14}$$

$$\sigma_2 = \sqrt{\frac{2}{3}} \left\{ \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\} \tag{3.15}$$

$$\sigma_3 = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix} \right\}, \tag{3.16}$$

with which we can write all density cubes for the qubit as

$$\rho = \frac{1}{2}(\sigma_0 + \mathbf{x} \cdot \boldsymbol{\sigma}). \tag{3.17}$$

This shows that the density cube description cannot add anything to the quantum description in the qubit scenario. This was expected, as there are no three distinct states which could produce genuine interference.

3.2.2. The qutrit case

We have hermiticity conditions analogous to the qubit case, with ten distinct real parameters of the types ρ_{iii}, ρ_{iij} as well as a complex parameter ρ_{123} involved.

This latter entry of the density cube (and the permutations of 123) have no equivalent in the quantum case, and hence we expect that if $\rho_{123} = 0$ (as well as its permutations), we could map the density cube ρ_{ijk} to the quantum qutrit density matrix ρ_{ij}:

$$\rho_{iij} = \frac{1}{\sqrt{3}} \rho_{ij} = \frac{1}{\sqrt{3}} \rho^*_{ji} \quad (i \neq j) \tag{3.18}$$

$$\rho_{iii} = \rho_{ii}, \tag{3.19}$$

which, luckily, also preserves the scalar product.

We now turn to cases where $\rho_{123} \neq 0$, meaning genuine third-order interference is involved. We consider a limited class[10] of density cubes, which fulfil the positivity condition:

$$\rho_1 = \left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2\sqrt{3}} \\ 0 & \frac{1}{2\sqrt{3}} & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & \frac{1}{2\sqrt{3}} \\ 0 & \frac{1}{2} & 0 \\ \frac{1}{2\sqrt{3}} & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & \frac{1}{2\sqrt{3}} & 0 \\ \frac{1}{2\sqrt{3}} & 0 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix} \right\} \tag{3.20}$$

$$\rho_2 = \left\{ \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{\omega}{2\sqrt{3}} \\ 0 & \frac{\omega^*}{2\sqrt{3}} & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & \frac{\omega^*}{2\sqrt{3}} \\ 0 & 0 & 0 \\ \frac{\omega}{2\sqrt{3}} & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & \frac{\omega}{2\sqrt{3}} & 0 \\ \frac{\omega^*}{2\sqrt{3}} & 0 & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix} \right\} \tag{3.21}$$

$$\rho_3 = \left\{ \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{\omega^*}{2\sqrt{3}} \\ 0 & \frac{\omega}{2\sqrt{3}} & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & \frac{\omega}{2\sqrt{3}} \\ 0 & \frac{1}{2} & 0 \\ \frac{\omega^*}{2\sqrt{3}} & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & \frac{\omega^*}{2\sqrt{3}} & 0 \\ \frac{\omega}{2\sqrt{3}} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right\}, \tag{3.22}$$

where $\omega = e^{i2\pi/3}$.

[10]The complete characterization of the set is not yet known.

The states ρ_i are orthogonal, $(\rho_i, \rho_j) = \delta_{ij}$; the quantum part of their density matrix can be obtained from the density matrix $\frac{1}{2}(\mathbf{1} - |e_i\rangle\langle e_i|)$, where the $|e_i\rangle$ form the standard quantum basis for the qutrit.

If we write the quantum state $|\psi\rangle$ as a vector with respect to the base kets e_i: $|\psi\rangle = (c_1, c_2, c_3)^T$, then we can write the corresponding density cube for the pure state $|\psi\rangle\langle\psi|$:

$$\rho^{(n)}_{iij} = -\frac{1}{2\sqrt{3}} c_i^* c_j, \quad i \neq j \tag{3.23}$$

$$\rho^{(n)}_{iii} = \frac{1}{2}(1 - |c_i|^2) \tag{3.24}$$

$$\rho^{(n)}_{123} = \frac{\omega^n}{2\sqrt{3}} \tag{3.25}$$

we can verify that positivity is preserved, as $(\rho^{(n)}(|\psi\rangle), \rho^{(m)}(|\phi\rangle)) = \frac{1}{4}(1 + |\langle\psi\phi\rangle|^2) + \frac{1}{4}\cos\frac{2\pi(n-m)}{3}$. It is not clear whether the entire group of transformations would lead to positive states.

3.3. A transformation for density cubes

3.3.1. Idea

Now that the class of ρ_i is defined and its positivity assessed, we may look at interesting transformations involving this class of density cubes.

A very simple transformation, which we will call T, simply maps the ρ_i to the e_i (the density cube representing the pure state $|e_i\rangle$ and vice-versa:

$$\boxed{T(\rho_i) = e_i, \quad T(e_i) = \rho_i.} \tag{3.26}$$

3.3.2. Matrix form

To assess the action of T on other density cubes, we will first define subbasis $E^{(i)}$ among the "hermitian" cubes:

$$E^{(n)}_{ijk} = \delta_{in}\delta_{jn}\delta_{kn} \quad n = 1,2,3 \tag{3.27}$$

$$E^{(4)} = \frac{1}{\sqrt{3}}\left\{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right\} \tag{3.28}$$

$$E^{(5)} = \frac{1}{\sqrt{3}}\left\{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\right\}. \tag{3.29}$$

If $\rho \in \text{span}(E^{(n)})$, we suppose $T(\rho) \in \text{span}(E^{(n)})$, $n = 1, \ldots, 5$. Therefore, we can write T as a 5×5 matrix, and the density cubes ρ_i and e_i as:

$$e_1 = (1,0,0,0,0)^T, \quad e_2 = (0,1,0,0,0)^T, \quad e_3 = (0,0,1,0,0)^T \tag{3.30}$$

$$\rho_1 = \frac{1}{2}(0,1,1,1,1)^T, \quad \rho_2 = \frac{1}{2}(1,0,1,\omega^*,\omega)^T, \quad \rho_3 = \frac{1}{2}(1,1,0,\omega,\omega^*)^T. \tag{3.31}$$

Now, requiring that $Te_i = \rho_i$ and furthermore imposing the condition that T has to be unitary, we obtain the representation of T in the $E^{(n)}$ basis:

$$T = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & \omega^* & \omega \\ 1 & 1 & 0 & \omega & \omega^* \\ 1 & \omega & \omega^* & 1 & 0 \\ 1 & \omega^* & \omega & 0 & 1 \end{pmatrix} \tag{3.32}$$

it is clear that T is symmetric, unitary and thus $T^2 = \mathbb{1}$. It also is clear that $T(\rho_i) = e_i$, thus it captures our initial intuition.

3.4. Violating the quantum bound

Using the matrix form of T, given in (3.32), we can derive a violation of the quantum bound of the 4-time Leggett-Garg inequality.

We devise a dichotomic measurement (A) of the quantum part of the density cube, which has as eigenvalue $+1$ for the eigenket $|e_1\rangle$ and -1 for the eigenkets $|e_2\rangle$ and $|e_3\rangle$.

We then start with e_1 as starting density cube, and can apply measurements at two out of four times for each run of the experiment. In between the measurements, the matrix T is applied, see figure 3.1.

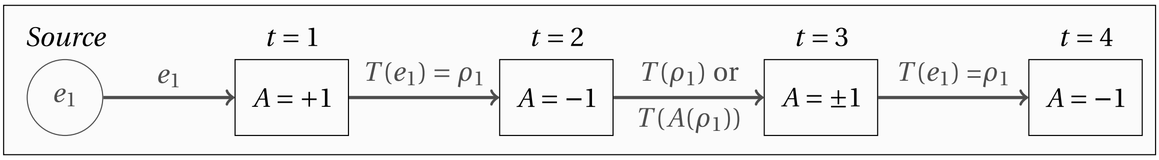


Figure 3.1: *Leggett-Garg setup with the T-transformation for density cubes applied at each time step. For each run only measurements at two times are conducted; at the two remaining times, the system is left alone. The measurement at $t = 1$ always yields $+1$ (if made), and does not change the state. The measurement at $t = 2$ always yields -1 and outputs the state $A(\rho_1)$ (either e_2 or e_3 with the same probability), if made. The measurement at $t = 3$ yields $+1$ (and results in e_1) if* no *measurement was made conducted at $t = 2$, and else either $+1$ or -1 with same probability (the outcome is irrelevant, as already two measurements have then been made). The measurement at $t = 4$ always yields -1 if only one measurement was carried out before (i.e. in all relevant cases).*

Let us consider Tsirelson bound for the following Leggett-Garg inequality:

$$C_{23} + C_{13} + C_{24} - C_{14} \leq 2\sqrt{2} \quad \text{(quantum)}. \tag{3.33}$$

We can easily show that, using the T transformation in the setup of figure 3.1, the correlators are $C_{14} = -1$, $C_{13} = 1$, $C_{24} = 1$ and $C_{23} = 0$, whence:

$$C_{23} + C_{13} + C_{24} - C_{14} = 3 \quad \text{(density cube)}. \tag{3.34}$$

It therefore seems as if the density cube theory could achieve potential stronger correlations than in quantum mechanics, at least in the temporal scenario. Furthermore, it also seems as though it maintains the quantum theory as a special case, making it a potential generalization of it. We will see why this optimistic picture is tarnished in the next chapter.

4. Assessing the density cube theory

This chapter will be devoted to a critique of the density cube (and similar higher order theories). The first section will review the possible interpretations of the T-transformation in the standard quantum framework, the second section will show the limitations of the T-transformation, introduced in the last chapter.The third section consists of a proof that higher order interference theories cannot be an adequate generalization of quantum mechanics. In the fifth section, we will see how to use these results to interpret T. In the last section, we will review the the connections between signalling and a violation of the temporal Tsirelson bound and present a density cube transformation allowing to saturate the logical bound of the 4-correlator Leggett-Garg inequality.

4.1. Interpretation of third-order interference the standard quantum framework

Using Sorkin's classification of theories (section 3.1.2), we can make more sense of how third-order interference differs from usual quantum interference. The usual quantum scenario (see section 2.4) is that the correlators are given by $\langle A_1 A_2\rangle = \mathrm{tr}[1/2\{A_1, A_2\}\rho]$ in the temporal case and $\langle AB\rangle = \mathrm{tr}[(A\otimes B)\rho]$ in the spatial case. If there are four operators A_1, A_2, A_3, A_4 obeying $A_i^2 = \mathbb{1}$ then the correlators between the operators cannot violate the Tsirelson bound $2\sqrt{2}$ either for the Leggett-Garg or the CHSH inequality, as we have seen in section 2.4.

There are three ways to describe a violation of the Tsirelson bound (achieved by the T transformation of density cubes, see section 3.4), while remaining in the standard quantum framework. The first one is to have five instead of four operators. The transformation means that one operator (e.g. A_3) depends on the previous settings. We have A_3 if the previous measurement was done at $t = 1$ (or it is itself the first) and A_3' if the previous measurement was done at $t = 2$. Therefore the sum of correlators really should read $\langle A_1, A_3\rangle + \langle A_1, A_4\rangle - \langle A_2, A_3'\rangle + \langle A_2, A_4\rangle$ which is obviously not bound by $2\sqrt{2}$. However, this really consists in describing a different setup altogether, where the third measurement is not always the same, so it is a counter-intuitive description. It may however reflect that although the experimental setups are A_3 and A_3' are *thought* to be the same, there is some kind of hidden dependency on the input state.

Another way to interpret the stronger correlation is to modify the correlators to include a contribution apart from the scalar product (or trace): $\langle A_1 A_2\rangle = \mathrm{tr}(1/2\{A_1, A_2\}\rho) + I_3^{A_1} I_3^{A_2}$, where $I_3 = I_3(1,2,3)$ reflects the third-order interference measurement made by the operator. To obtain the correlations of section 3.4, one would have $I_3^{A_1} = 0$, $I_3^{A_4} = 0$, $I_3^{A_2} = 1$ and $I_3^{A_3} = 1$. This means postulating an *ad hoc* entity to supplement ordinary quantum correlators, an intuition that will be the driving force of higher order interference theories using the "second strategy", see section 4.3.3.

The third way to achieve the correlations is roughly the same as the second, as the equations are the same, yet it is based on a different interpretation. Here, one does not keep the eigenvalues a_i of A_i bounded by one, which also means that $A_i^2 = \mathbb{1}$ does not hold any more. One can (following section 2.4) identify each of the observables to a vector, and the correlators as scalar products. To achieve the correlators of 3.4, one needs to have two vectors of length $\sqrt{2}$: $\mathbf{a_1} = (0,1,0)$, $\mathbf{a_2} = (0,-1,1)$, $\mathbf{a_3} = (0,1,1)$ and $\mathbf{a_4} = -\mathbf{a_1}$. This extra component in z-direction is equivalent to the interference term I_3 in the last interpretation, but here it is explicitly included in the scalar product. The major problem with this formulation is that it can readily be interpreted as experimental outcomes (of $\mathbf{a_3}$ and $\mathbf{a_2}$) are $\pm\sqrt{2}$ rather than ± 1, which is not what the experimental setup implies.

All three interpretations can lead to the same correlations (and saturate the logical bound), yet the first one and the two last ones seem to have a very different meaning. I will explain why the first interpretation is (even if it is very unintuitive) to be favoured, in section 4.4.3.

4.2. Expanding T to two particles

In this section, we will investigate the generalization of T to a two-particle system, and the possibility to violate the quantum mechanical bound for the CHSH inequality by using it.

It will be shown that the most natural generalization of the quantum part of T is a positive, but not complete positive map, and if we circumvent this property, it is still impossible to violate quantum bounds in the spatial case, if we consider that the observables of the observers commute with each other.

4.2.1. Two particles and augmented basis

The initial objective was to express the 3-level, 2-particle state $|\psi^+\rangle = \frac{1}{\sqrt{3}}(|00\rangle + |11\rangle + |22\rangle)$ state the basis of tensor products of $E^{(i)} \otimes E^{(j)}$ given in 3.3. However the basis is not sufficient to achieve this, so additional elements representing the off-diagonal terms, are required.

I therefore introduced six new basis elements, labelled $E^{(6)}$ to $E^{(11)}$, which represent standard quantum correlations, for instance $E^{(6)} = |0\rangle\langle 1|$, $E^{(7)} = |1\rangle\langle 0|$, $E^{(8)} = |1\rangle\langle 2|$, $E^{(9)} = |2\rangle\langle 1|$, etc. Using these elements, it is possible to write the the state ψ^+ as $\frac{1}{3}\sum_{i\neq 4,5}^{11} E^{(i)} \otimes E^{(i)}$.

4.2.2. Effect on off-diagonal elements

The problem is that T in its original formulation (3.32) does not include effects on off-diagonal elements. For the purpose of examining two-particle-correlators, it will be easier to first use a representation for T that is restricted to its *measurable* effects, meaning those on the quantum part, denoted by T_{QM}. Surprisingly, a very simple generalization of it can still be given, knowing how it maps the base elements e_1, e_2 and e_3:

$$\boxed{T_{QM}(\rho) = \frac{1}{2}(\mathbb{1}_3 - \rho).} \tag{4.1}$$

This form reminds us of a *universal quantum NOT gate* (in the qubit case), introduced by Bužek et. al., who show that such a gate cannot be constructed for arbitrary input qubits [8]. This suggests that this map as well is impossible (if we assume it transforms purely quantum mechanically), although it is positive and trace-preserving.

We suppose that the Hilbert space of a composite system is the tensor product of the Hilbert spaces of the constituent systems. This requirement is natural in quantum mechanics (see section 2.1), but not necessarily for density cubes. It is not clear how to describe a system of several qutrits in the latter formalism, therefore we investigate the usual tensor product case. We show that under these assumptions *complete positivity* is not fulfilled by T_{QM}, making it a non-physical transformation.[11] Consider the transformation $\mathbb{1}_3 \otimes T_{QM}$, acting on the state $|\psi^+\rangle\langle\psi^+|$ (recall $|\psi^+\rangle = \frac{1}{\sqrt{3}}(|00\rangle + |11\rangle + |22\rangle)$):

$$(\mathbb{1}_3 \otimes T_{QM})|\psi^+\rangle\langle\psi^+| = \sum_{ij}^{3} |i\rangle\langle j| \otimes T_{QM}(|i\rangle\langle j|). \tag{4.2}$$

now it clear from (4.1) that $T_{QM}(|i\rangle\langle i|) = 1/2(\mathbb{1}_3 - |i\rangle\langle i|)$, however, for $i \neq j$: $T_{QM}(|i\rangle\langle j|) \neq 1/2(\mathbb{1}_3 - |i\rangle\langle j|)$, but rather $T_{QM}(|i\rangle\langle j|) = -|i\rangle\langle j|/2$.

We can now come back to the form of T, relative to the augmented base E_i, in which $\psi^+ = \frac{1}{3}\sum_{i\neq 4,5}^{11} E^{(i)} \otimes E^{(i)}$, because we know the action of T on the off-diagonal elements $|i\rangle\langle j|$ $(i \neq j)$, which are represented by $E^{(6)}$ to $E^{(11)}$. Therefore, we can write T', the natural generalization of T to arbitrary states (matrix form with respect to the subbasis $E^{(i)}$):

[11] Although the claim that complete positivity is a necessary condition for meaningful transformations has been challenged [27, 33] complete positivity will, for the purpose of this thesis, be upheld as a necessary requirement.

$$T' = \frac{1}{2}\begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & \omega^* & \omega & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & \omega & \omega^* & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \omega & \omega^* & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \omega^* & \omega & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \tag{4.3}$$

it is clear that T' is not unitary any more and $T'^2 \neq \mathbb{1}_{11}$, however the upper left part of T'^2 is still $\mathbb{1}_5$ and unitary.

In the basis E_i the tensor product[12] $\mathbb{1}_{11} \otimes T'$ can readily be computed, as well as the expectation value of ψ^+ in this representation. If we complete this (tedious) calculation, we obtain:

$$(\psi^+)^\dagger \cdot (\mathbb{1}_{11} \otimes T') \cdot \psi^+ = -\frac{1}{3}, \tag{4.4}$$

which proves that the T' (and therefore T, as given in (4.1)) is not a completely positive map.

Another way to show this, is to stay with the usual representation of T, as given in (4.2), and take the expectation value of $|\psi^+\rangle$. Again:

$$\langle\psi^+| \left[(\mathbb{1}_3 \otimes T)\,|\psi^+\rangle\right] \langle\psi^+|\,|\psi^+\rangle = \langle\psi^+| \sum_{ij}^{3} |i\rangle\langle j| \otimes T(|i\rangle\langle j|)\,|\psi^+\rangle = -\frac{1}{3}. \tag{4.5}$$

To conclude this study of the complete positivity of (4.1), it may be of interest to take a look at the best *approximation* of the universal NOT gate. It consists (for the qubit) in measuring the initial state, in an arbitrary basis, then rotating the measurement result to the orthogonal state. Repeating this procedure many times with a different initial state, one obtains:

$$\mathrm{NOT}_{QM}(\rho) = \frac{2}{3}\rho_\perp + \frac{1}{3}\rho = \frac{2}{3}\mathbb{1}_2 - \frac{1}{3}\rho \quad \text{(qubit)}. \tag{4.6}$$

This can easily be generalized to any dimension n:

$$\mathrm{NOT}_{QM}(\rho) = \frac{2}{3}\rho_\perp + \frac{1}{3}\rho = \frac{4}{3}\frac{\mathbb{1}_n}{n} - \frac{1}{3}\rho \tag{4.7}$$

$$\stackrel{n=3}{=} \frac{4}{9}\mathbb{1}_3 - \frac{1}{3}\rho \tag{4.8}$$

with $\rho_\perp = \mathbb{1}_n/n - \rho$. For the qutrit, this is the same as (4.1), only with a weight reduced in magnitude for ρ. It is straightforward to show (using an equation similar to (4.5)) that any negative weight of higher absolute value than $1/3$ for ρ destroys the property of complete positivity.

[12] Remember that this still represents the action on a three-level system, the additional base elements are not independent degrees of freedom!

4.2.3. Effect on off-diagonal elements, second try

There may still be an option to "save" the complete positivity of T. We could simply reject the expression given in (4.1), and thus the resulting T' and simply *choose* a convenient way of expanding T to off-diagonal elements.

When evaluating the complete positivity of T' in (4.4), it is striking that the negative value comes from the off-diagonal elements mapped (up to a factor) to themselves ($T(|i\rangle\langle j|) = -|i\rangle\langle j|/2$, where $i \neq j$): one could add any proportionality constant $\alpha > 0$: $T(|i\rangle\langle j|) = -\alpha|i\rangle\langle j|$, without being able to save complete positivity. So, in any case, what is needed is $\alpha = 0$.

Now let us come to mapping of the off-diagonal elements to off-diagonal elements other than themselves. We could, for instance, have the following expanded version $\tilde{T}$:

$$\tilde{T} = \frac{1}{2}\begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & \omega^* & \omega & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & \omega & \omega^* & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \omega & \omega^* & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \omega^* & \omega & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 & 1/2 & 1/2 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 & 1/2 & 1/2 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 1/2 & 1/2 & 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 1/2 & 1/2 & 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 1/2 & 1/2 & 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/2 & 1/2 & 1/2 & 1/2 & 0 & 0 \end{pmatrix}, \tag{4.9}$$

where $\tilde{T}$ is again not unitary and $\tilde{T}^2 \neq \mathbb{1}_{11}$, but the upper left part of $\tilde{T}^2$ is still $\mathbb{1}_5$. Here, we map each off-diagonal element to the remaining ones (with a factor 1/4 to keep positivity). This transformation is completely positive.

Remark. *It should be noted that choosing the effect on the off-diagonal elements more or less independently of one on diagonal elements is highly problematic for $\tilde{T}$. We will ignore this for now, and see what can be done with $\tilde{T}$.*

4.2.4. Violating quantum mechanics in the CHSH scenario?

Ignoring the difficulties mentioned above, we now have a candidate $\tilde{T}$ for the use in the (spatial) CHSH scenario, consisting of two observers, two measurement setups and two outcomes per setup. Here, as we initially consider a qutrit, we group the results 2 and 3 together to "−1" and 1 to "+1", as it was done in the temporal scenario using T (see section 3.4). The question is: Can the Tsirelson bound ($2\sqrt{2}$) be violated by $\tilde{T}$ as it has been in the temporal case by T?

We numerically tested this scenario for different pure (entangled and separable) initial states, different transformations based on $\tilde{T}$, including $\mathbb{1}\otimes\tilde{T}$, $\tilde{T}\otimes\tilde{T}$, $\mathbb{1}\otimes((1-\epsilon)\mathbb{1}+\epsilon\tilde{T})$ with all possible measurement operator combinations A, A', B, B'. Never was it possible to achieve a violation of the Tsirelson bound; worse, it appears that the bound can only be saturated, when no $\tilde{T}$ is involved at all (although we have no proof for this). So there are good reasons to believe that $\tilde{T}$ does not show the necessary features to violate the quantum bound in the CHSH scenario.

Spatial inequalities for the qutrit, taking into account the three possible outcomes [12, 19] were also probed, without managing to achieve stronger than quantum correlations.

We can characterize T_{QM} as in (4.1), as the quantum NOT gate. The problem of complete positivity arises only for a *universal* gate, once something about the state is known, there can be such a transformation.[13] So we *could* conceptualize[14] that T can be realized by using only quantum mechanical operations, together with knowledge of the input state, it is as if $T(\rho) = T_\rho(\rho)$, where the index means the transformation to be applied depends on the input state. With this I mean that one could realize the transformation T in the following way: the particle or some other "hidden carrier of information" carries the information about the incoming state into the device that is supposed to perform the transformation T. The device reads out this information and prepares accordingly ordinary quantum operation T_ρ that depends on the incoming state. Note that the devices prepares *different* transformation for different incoming states, although from observer's point of view, all of them are associated to a single "switch position" on the device.

It is crucial that in the Leggett-Garg scenario, the quantum bound applies only if the involved transformation does not depend on the state, else the condition that the measurement setups are independent of each other breaks down. In the CHSH scenario, the use of having additional knowledge of the state is that it allows signalling of the result of one part to the other part. It seems however, that T does not recover sufficient information to allow this signalling resource to be sufficient for breaking the Tsirelson bound, possibly pointing to a deep difference between spatial and temporal inequalities.

4.2.5. Summary

Let us resume the findings of this section: there are severe problems with T as introduced in section 3.3: the most natural generalization to off-diagonal elements is not completely positive, and a possible solution to this introduces base dependence, breaking isotropy.

If we were to accept this mapping, it would need to be understood as being state dependent: T would be understood as a set of usual quantum transformations together with a demon, capable of non-destructively determining the incoming state, selecting the right transformation according to the input. Such a demon violates the assumptions of the Leggett-Garg scenario (the measurement setups are no longer independent) and, in principle also the no-signalling condition of the spatial CHSH scenario. However, it seems that as T is unable to allow signalling of any useful information to violate the Tsirelson bound in the spatial case.

4.3. General incompatibility of higher order interference terms with quantum mechanics

In this section, we will see that any theory making use of non-zero interference terms of a higher order than quantum mechanics cannot include quantum mechanics as some kind of limit, or will otherwise imply negative probabilities.

4.3.1. Requirements

First, a shortened version of quantum mechanical description shall be given, a working summary of the longer account given in section 2.1:

Definition 4.1. *To describe an "ordinary quantum system", the following conditions have to be met:*

1. *There is a state Hilbert space $\mathscr{H}$, containing pure state kets.*

2. *There is a density operator $\rho \in L(\mathscr{H})$, which is positive and has trace one.*

[13] For example with the qubit $a|+\rangle + b|-\rangle$, if we know that a and b are real [8].

[14] This does not mean that T does not have formalizations which are independent of ρ, the counterexample is (4.1) itself. However, if we want complete positivity in the framework of the usual tensor product, we cannot chose such a formalization, and therefore we can settle for state dependency.

3. *The possible quantum operations (e.g. unitary transformation, POVM, partial trace) map density operators on one Hilbert space to density operators on another (possibly the same one) space* $L(\mathcal{H}_1) \to L(\mathcal{H}_2)$. *They are therefore required to be completely positive and trace-preserving.*

There are two "natural" requirements for a physically interesting higher-order interference theories. We should ask that it adds something new to standard quantum theory and that it coincides with the latter in describing the world:

Requirement 1. *It must include quantum mechanics as a special case – when the higher order terms vanish, the experimental results attainable with the dynamics of definition 4.1 must be "recovered".*

Requirement 2. *It has to predict experimental results which are in contradiction with the dynamics of definition 4.1. In other words, there must be at least one* experimentum crucis *differentiating ordinary quantum mechanics from the more general theory.*

We will now look at different strategies, and evaluate their success at fulfilling both requirements. I will show that none of them can do so.

4.3.2. First strategy

There are two main strategies to implement higher order interference. The first one consists in devising a *non-QM operation* – i.e. the third order interference term is used only to allow a specific transformation, but keeping the state space as in quantum mechanics – density operators as description of systems. It does not interfere with the trace or measurement process itself, which is still considered as purely quantum mechanical. To be able to produce experimental results, like temporal correlations, which contradict quantum behaviour there must exist at least one) non-quantum transformation.

Recalling that every quantum operation is, by definition a positive, trace-preserving map, it is clear that any "genuine higher-order" and non-quantum transformation is will annihilate the probability interpretation of the trace, where the latter are negative and/or do not sum up to one. Thus the theory will not be able to maintain quantum mechanics as a special case and fails to fulfil the first requirement.

4.3.3. Second strategy

The second strategy seems more promising. It consists in extending the density operator itself to include some terms reflecting the higher order interferences. This can be done in a variety of ways.[15]

When one increases the degrees of freedom available to ρ there are again two options. One is to keep the quantum mechanical scalar product ($\mathcal{H}^* \times \mathcal{H} \to \mathbb{C}$) as way to calculate probabilities, with *added* terms in case of a higher order interference:

$$\boxed{(\rho, \sigma) = \mathrm{tr}[\rho_{QM} \sigma^*_{QM}] + \rho_{\neg QM} \sigma^*_{\neg QM},} \tag{4.10}$$

where ρ and σ are density operators of the extended theory, ρ_{QM} the quantum part and $\rho_{\neg QM}$ represents (in which way exactly is irrelevant) the non-quantum part of ρ.

This is basically equation (3.7) for the trace of a density cube. Now it is clear that $|(\rho, \sigma)| \leq 1$ therefore any non-quantum correlation can only be achieved with mixed states. A non-quantum-mechanical transformation achieving this is the T transformation – it creates $\rho_{\neg QM}$ at the expense of mixing ρ_{QM}.

This first step seems "harmless" in a way, as the mixing on ρ_{QM} could also be achieved through ordinary quantum operations. The difference is that there is a "memory" of the original state left in

[15] Either by increasing the size of the density matrix or by introducing additional indices and defining the density operator as a map $\rho : \mathcal{H} \times \ldots \times \mathcal{H} \to \mathcal{H}$, i.e. making ρ a tensor of rank > 2. The latter formulation is used in the density cube theory, see section 3.2.

the form of $\rho_{\neg QM}$. The question is, can any meaningful reversible operation be devised that does not violate positivity of the scalar product. We shall prove that, under a limited number of reasonable conditions, no such reverse operation be conceived, nor even can we devise a consistent operation to obtain $|\rho_{\neg QM}| > 0$ from a purely quantum sate. Thus, no theory using (4.10) can fulfil the requirements 1 and 2.

Lemma 4.1. *Given a higher order interference theory of type* (4.10)*, and of order purely n (i.e. there is* only *added n-interference), for a n-level quantum state ρ_{QM} there is only one additional complex degree of freedom: $\rho_{\neg QM} \in \mathbb{C}$.*

Proof. This follows immediately from Sorkins classification of theories [35, 36]; as seen in section 3.1.2 the additional interference term can is always described by a single (potentially complex) number. □

Remark. *We will furthermore require this degree of freedom to be a physically meaningful quantity, and therefore $|\rho_{\neg QM}|$ to transform as a* scalar.

Definition 4.2. *Quantum mechanical mixing operations are maps $\rho \mapsto \rho'$, with $\rho' = \alpha\rho + (1-\alpha)\tilde{\rho}$ (where $\tilde{\rho}$ and $\alpha \geq 0$ are fixed.)*

Lemma 4.2. *Given a higher order interference theory of type* (4.10)*, and of order purely n; given a purely quantum mechanical initial state ρ (i.e. $\rho_{\neg QM} = 0$), the only one class of transformations resulting in $|\rho_{\neg QM}| > 0$ is a mixing, given by:*

$$\rho_{QM} \mapsto \alpha\rho_{QM} + (1-\alpha)\frac{\mathbf{1}_n}{n} \quad 0 \leq \alpha \leq 1, \tag{4.11}$$

whence, clearly, the following bound applies:

$$|\rho_{\neg QM}|^2 \leq 1 - \left(\alpha^2 + \frac{2\alpha(1-\alpha)}{n}\right) - \frac{(1-\alpha)^2}{n} = 1 - \alpha^2 + \frac{\alpha^2 - 1}{n}. \tag{4.12}$$

Proof. The only class of quantum operations potentially reducing the $\mathrm{tr}[\rho_{QM}^2]$ are mixing operations, given by definition 4.2. Therefore, a transformation leading to $|\rho_{\neg QM}| > 0$ must be a mixing.

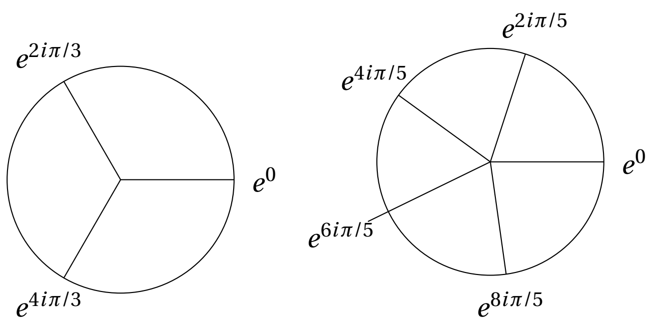
Now suppose we mix the initial state with any other state (than the fully mixed one), which is not invariant under rotation and obtain $\rho_{\neg QM} \neq 0$. Then $|\rho_{\neq QM}|$ term would then not be invariant under unitary transformation: it would *not transform as a scalar*, which we required by the remark following lemma 4.1. The bound follows from obvious reasons of normalization, given that the initial state is pure ($\mathrm{tr}[\rho_{QM}^2] = 1$). □

Lemma 4.3. *Given a higher order interference theory of type* (4.10)*, and of order purely n; given a basis $|\psi_j\rangle$ for the n-dimensional Hilbert space, each pure state $\rho_{QM} = |\psi_j\rangle\langle\psi_j|$ undergoing transformation* (4.11) *will result in a higher order interference term of the same absolute value (without loss of generality, we choose it to saturate the bound* (4.12)*), rotated by $2\pi/n$ in the complex plane:*

$$|\psi_j\rangle\langle\psi_j| \mapsto \alpha|\psi_j\rangle\langle\psi_j| + (1-\alpha)\frac{\mathbf{1}_n}{n} \quad 0 \leq \alpha \leq 1, \tag{4.13}$$

$$\rho_{\neg QM} \mapsto e^{i\theta}\left(1 - \alpha^2 + \frac{\alpha^2 - 1}{n}\right)^{1/2} e^{i\frac{2\pi j}{n}}, \tag{4.14}$$

where θ is an arbitrary global phase, which can be disregarded in the subsequent considerations.



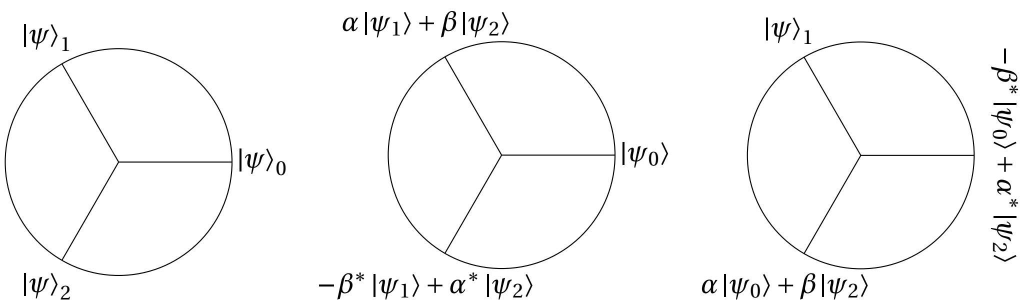
(a) $n = 3$ (b) $n = 5$

Figure 4.1: *Complex roots for $n = 3$ and $n = 5$. They correspond (up to the amplitude) to the possible values for $\rho_{\neg QM}$ when mixing pure base kets, as in* (4.14).

Proof. Given an initial fully mixed quantum state $\rho_{QM} = \mathbf{1}_n/n$ with $\rho_{\neg QM} = 0$. The transformation (4.11) is in this case independent of α, therefore no new higher order interference term can be created. Furthermore, taking $\mathbf{1}_n/n = \sum_j^n |\psi_j\rangle\langle\psi_j|/n$ because of linearity of the transformation and of rotation invariance transformed each pure state will result in a higher order interference term of the same absolute value. Therefore, the terms have to be placed on the complex plane so that the vectorial sum of all of them gives zero, which can only be achieved by having a phase shift of $e^{i2\pi/n}$ between each $\rho_{\neg QM}$ obtained by a transformation of subsequent pure states $|\psi_j\rangle\langle\psi_j|$ (see a graphical representation in Figure 4.1). □

Lemma 4.4. *Given a higher order interference theory of type* (4.10)*, and of order purely n, there is no consistent map obeying the conditions of lemma* 4.3.

Proof. Having a base $|\psi_j\rangle$, consider the change of all but one of the basis kets. The transformation of the vector which has remained the same must be mapped to the same complex root, for consistence. Hence all other basis vectors must fall on the same points as for the previous base (possibly in different order), as the angle between each new pair must be the same as before. One can repeat this procedure an arbitrary number of times[16] – this proves that all *pure* states are mapped on the n roots only (see Figure 4.2).



(a) Initial base (b) Rotate around $|\psi\rangle_0$ (c) Rotate around $|\psi\rangle_1$

Figure 4.2: *How base changes affect the position of $\rho_{\neg QM}$ on the complex circle (for $n = 3$). Because one base ket can alway be kept fixed, there are only n possible positions for $\rho_{\neg QM}$, if the initial state is pure. Note that any rotations can be made, as long as $|\alpha|^2 + |\beta|^2 = 1$.*

[16] Every pure state can be obtained by a sequence of rotations in two-dimensional subspaces [31].

It would be fatal to have an inconsistent mapping, i.e. orthogonal kets mapped to the same root.[17] The only way to avoid this is to assign each initial base vector a 90°-cone around it, and specify that all vectors in it will always be mapped to the same vector. However, this is not base invariant, and repeating this for different bases will result in different cones, so there is no consistent mapping possible. If one uses just the cones of one particular basis, then the vectors on the opposite faces will be (arbitrarily close to) orthogonal too (see Figure 4.3), therefore rendering a consistent mapping highly singular. □

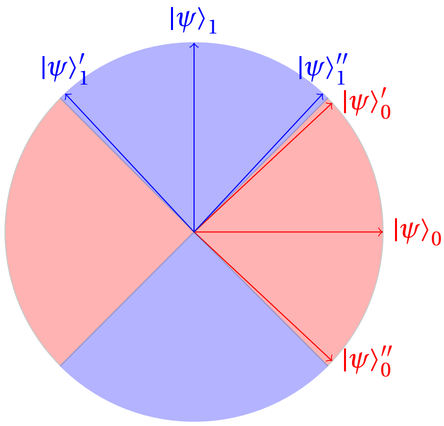


Figure 4.3: *Representation of a 2-d subspace of the n-dimensional Hilbert space. By rotating, and keeping the other axes fixed, we can chose how to map the rotated vectors to the two possible values $\rho_{\neg QM}$ on the complex plane. To avoid having mapping orthogonal pairs to the same point on the complex plane, one can chose to have a rule for mapping: vectors in the blue cone will be mapped to one point, and the ones in the red cone to the other one. Unfortunately, one can have vectors arbitrarily close to being orthogonal ($|\psi\rangle'_1$ and $|\psi\rangle''_1$ for example) mapped to the same point. Equally, tow arbitrarily close vectors (eg $|\psi\rangle''_1$ and $|\psi\rangle'_0$) will be mapped to two different points.*

Theorem 4.5. *There cannot be any non-quantum operation derived from a higher order interference theory of order purely n obeying* (4.10) *that satisfies the requirements 1 and 2.*

Proof. From lemma 4.4 it is clear that there can be no consistent non-quantum operation that satisfies lemma 4.3. Hence requirement 2 cannot be fulfilled at the same time as requirement 1 for theories obeying the modified scalar product (4.10). □

Remark. *An information theoretic argument could possibly construct a direct contradiction of lemma 4.1, which gives one complex degree of freedom for $\rho_{\neg QM}$ a potential reverse mapping from $\rho_{\neg QM}$ to a genuine quantum state, which would need $n-1$ complex degrees of freedom. It would provide for a more elegant proof of theorem 4.5 and may be worth some further investigation.*

Corollary 4.6. *Theorem 4.5 holds for any general higher order interference theory of order n obeying* (4.10)*, also if it includes lower order interference terms ($n-1$, $n-2$ etc.).*

Proof. This can easily be shown through induction: by applying theorem 4.5 to $n = 3$ to show there can be no pure third-order interference first. We then repeat the argument for a theory of an interference

[17] Not only would this mean there can be no meaningful back-transformation, it would also, more importantly, *violate the property that the transformation of an already fully mixed state does not produce a non-quantum part.*

order purely $n = 4$ (as $n = 3$ was shown to be impossible), for which we use a state with four degrees of freedom. We can repeat this step as often as needed – therefore, the theorem holds for any n. □

4.3.4. Third strategy

The last strategy to include higher order interference terms is to abandon the quantum mechanical scalar product as primary object and replace it with a multilinear form ($\mathscr{H} \times \ldots \times \mathscr{H} \to \mathbb{C}$) of, at least, the order of the required interference.

This seems like the most natural generalization of quantum mechanics, as it extends the very core of the quantum theory, the scalar product from which experimental probabilities are recovered. I will treat the approach in two separate parts, multilinear forms of odd order firstly and of even order secondly.

Odd multilinear forms

Proposition 4.7. *A multilinear form of odd order cannot be positive. Therefore, the quantum scalar product cannot be recovered from it as a limit.*

Proof. Relying on Qi's generalization of eigenvalues to tensors of arbitrary order [30], it is clear that one can only talk of positive semidefiniteness of a tensor when it is of even order.

Suppose an m-linear (m odd) form defined by F were positive: take a vector $\mathbf{x}$ (components x^i) for which the multilinear form $\mathbf{x}F\mathbf{x}^{m-1} = x^{i_1} F_{i_1}^{i_2 \ldots i_m} x_{i_2} x_{i_3} \cdots x_{i_m} > 0$, and supposedly represents a probability. Then the transformation $\mathbf{x}' = -\mathbf{x}$ (a basic reflection in the state space which has no physical effect in quantum mechanics) leads to $\mathbf{x}' F \mathbf{x}'^{m-1} < 0$, meaning positivity is not preserved. Odd multilinear forms can therefore give no meaningful account of the standard scalar product. □

Even multilinear forms Even multilinear forms are more challenging, as they can be positive. The following argument relies on the simplest generalization, using a 4-linear form and accordingly the density operator is a tensor of order 4 ($\rho \in L(\mathscr{H} \times \mathscr{H})$); higher orders are analogous in structure. The generalization to a 4-th order tensor implies the 4-linear form of which little is yet known:

$$(\cdot,\cdot,\cdot,\cdot) : (L(\mathscr{H} \times \mathscr{H}))^4 \to \mathbb{C} \tag{4.15}$$

$$(\rho,\rho,\rho,\rho) \leq 1 \quad \forall \rho \in L(\mathscr{H} \times \mathscr{H}). \tag{4.16}$$

Because of requirement 1 we would need to recover the standard quantum scalar product from formula. Symmetry suggests to choose $(\rho,\rho,\sigma,\sigma) = (\rho,\sigma)_{QM}$, at least when ρ and σ are devoid of higher order interference terms. We can write the 4-linear form as a factorizable term (which can be written as a product of quantum scalar products) and an additional non-factorizable 4-linear form $[\cdot,\cdot,\cdot,\cdot]$ that remains to be examined:

$$(\rho,\sigma,\tau,\xi) = \sqrt{(\rho,\tau)_{QM}(\sigma,\xi)_{QM}} + [\rho,\sigma,\tau,\xi], \tag{4.17}$$

therefore, for just two states:

$$\boxed{(\rho,\rho,\sigma,\sigma) = (\rho,\sigma)_{QM} + (\rho,\sigma)_{\neg QM}.} \tag{4.18}$$

Now in (4.18), the same structure as in the second strategy (see (4.10)) appears, in spite of the more general formalism. The experimentally accessible $(\rho,\rho,\sigma,\sigma)$ can be decomposed into a quantum and an additional higher order interference term, so theorem 4.5 applies here too.

The argument is the same for any even multilinear form that should generalize the scalar product. One can always separate it into a product of ordinary quantum scalar products and a non-factorizable term. Thus from theorem 4.5 one can conclude:

Corollary 4.8. *No multilinear form can be the foundation for a theory of higher order interference which satisfies the requirements 1 and 2.*

4.4. Reassessing the T-transformation

In the light of section 4.3 it is now possible to reassess the T transformation – where exactly the violation of the Tsirelson bound comes from and where the positivity is broken. I will examine the T transformation here as an example transformation of an explicit "second strategy" theory where the scalar can be expressed with (4.10), even if this formulation was not explicitly used in the first place.

4.4.1. First step – mixing

It was shown in section 4.3 that there cannot be a generalization of quantum mechanics to higher order theories while keeping the quantum limit. However, the T transformation seems to do just that.

Indeed, T fulfils requirement 2, but only at the expense of requirement 1. We showed in section 4.2.2 that the quantum part T_{QM} of the T transformation can most naturally be expressed as:

$$T_{QM}(\rho) = \frac{1}{2}(\mathbb{1}_3 - \rho) \tag{4.19}$$

This map, we then saw, is positive but not completely positive, and hence cannot be seen as a physically relevant quantum transformation.

Now look at the non-quantum part of T. Because it satisfies $T_{QM}(\mathbb{1}_3/3) = \mathbb{1}_3/3$, the non-quantum part of the transformation for each quantum base ket e_i has to have a phase difference of $2\pi/3$, as we saw in lemma 4.3. For the T-transformation of density cubes, this is the case: the resulting ρ_{123} is either (proportional to) $\pm\omega$ or to 1. We showed that this mixing cannot work base independently and have concluded that mapping two states with arbitrarily little overlap will be mapped to a *single* root. Therefore T is not physically plausible.

4.4.2. Second step – reverting to a pure state

Let us suppose that there *could* be a consistent mapping onto ρ_{123}. Then the reverse operation, outside of quantum mechanics, would be to "re-purify" the state (at least to some amount). However, there also seems to be a problem here. For any initial pure state, the resulting $\rho_{\neg QM}$ only can take three possible angles in the complex plane, yet one needs to recover three real degrees of freedom (the factors for all three base kets) for a reverse transformation to work as it does when applying T a second time ($T^2 = \mathbb{1}$).

However, the reverse transformation takes advantage of the highly curious nature of the "mixing" (4.1) itself, which sets the diagonal entry corresponding to the initial pure state to zero, thus providing an additional information storage in the quantum part of the state; the other degree of freedom results from considering only one base (e_1, e_2, e_3) and thus allows evading theorem 4.5 (obviously at the expense of requirement 1)

4.4.3. The best interpretation

From section 4.2.4, it is possible to clarify the three interpretations of T that were given in section 3.1. Given that no violation of the Tsirelson bound can occur in the spatial case, it seems clear that T does not directly lead to violating the condition on operators (that they square to $\mathbb{1}$ or can be represented as two-dimensional vectors with norm ≤ 1). Therefore, for me, the best interpretation is that

T is a transformation which has different forms depending on the input state: $T(\rho) = T_\rho(\rho)$ – imagine some kind of microscopic demon capable of (non-destructively) determining ρ and then modifying some parameters in the apparatus responsible for T according to the result. And while this can affect temporal correlations, it cannot affect spatial ones, because knowing the initial state in the spatial CHSH scenario is of no use in achieving stronger correlations.

4.5. Signalling and a stronger violation of the Tsirelson bound

4.5.1. Signalling

While signalling is obviously not prohibited in the temporal case (locality is not an issue), the *amount* of information that the experimentator can transmit to the next time by chosing at which times the first measurement has to take place may still be limited.

Following this intuition, Fritz [15] sets up an interesting bound for quantum signalling in the temporal scenario. He uses the following signalling quantities:

$$S_+ = P(+1,+1|1) + P(-1,+1|1) - P(+1,+1|2) - P(-1,+1|2) \tag{4.20}$$

$$S_- = P(+1,-1|1) + P(-1,-1|1) - P(-1,-1|2) - P(+1,-1|2) \tag{4.21}$$

where $P(+1,+1|1)$ is the conditional probability to obtain $+1$ twice given that the first setting is chosen for the first observation, and $S_+ + S_- = 0$ by virtue of probabilities summing up to one. Now the theorem established is:

Theorem 4.9 (Fritz' [15] Theorem 5.1)**.** *A signalling level* $S_+ \in [-1,1]$ *is quantum mechanical iff* $|S_+| \leq \frac{1}{2}$.

The proof that quantum mechanics $\Rightarrow |S_+| \leq 1/2$ is straightforward. The inverse direction is proven through the fact that the bound can be reached by QM and by the fact that the set of values for S_+ needs to be convex.

However, it is straightforward that the T transformation, while violating the Tsirelson bound, for each possible combination of settings, complies with the bound of theorem 4.9. Therefore, it is well possible to be within the bound for each pair of measurements, without respecting the Tsirelson bound on the whole; it seems that S_+ is not a very useful indicator of how “non-quantum” a behaviour is.

4.5.2. Stronger violation of the Tsirelson bound

Looking into the violation of the Tsirelson bound, achieved by T in (3.34), we see that there is still room for even stronger correlations. The question is, can we reach a violation even closer to the logical bound of four, or maybe can we even reach this bound, thus giving an account of the temporal equivalent of PR-boxes?

In turns out that the mapping $\hat{T}$ (written in matrix form with respect to the subbasis $E^{(n)}$ of density cubes) does the trick:

$$\hat{T} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 2 & 2 \\ 1 & 2 & 0 & -1 & -1 \\ 1 & 0 & 2 & -1 & -1 \\ 1 & 0 & 0 & 1 & -1 \\ 1 & 0 & 0 & -1 & 1 \end{pmatrix} \tag{4.22}$$

It is trace-preserving and maps $e_1 \mapsto \rho_1, \rho_1 \mapsto e_1, e_2 \mapsto e_2, e_3 \mapsto e_3$ (using the same base as in section 3.3), and retains the property $\hat{T}^2 = \mathbb{1}_5$, but it is not unitary [18].

[18] Unitarity in this context means having the length of the density cube vector stay the same; it is just a nice computational

If we repeat the thought experiment carried out with T, and replace it with $\hat{T}$ (see figure 4.4), then nothing changes in the experimental outcomes, except for $t = 3$, where the result is this time opposite of whatever measurement was made before (either $t = 1$ or $t = 2$, thus resulting in $C_{23} = 1$. All other correlators stay the same.

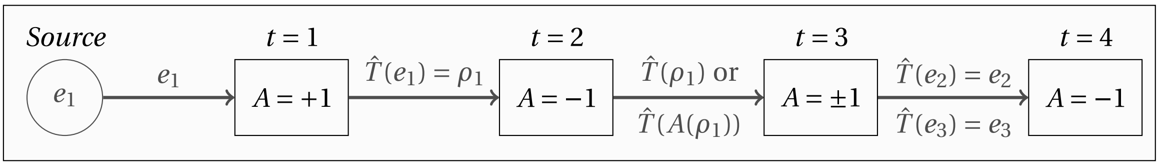


Figure 4.4: *Leggett-Garg setup with $\hat{T}$-transformation for density cubes. At each run only two measurements are made; at the two remaining times nothing is done. The measurement at $t = 1$ always yields $+1$ (if made), and does not change the state. The measurement at $t = 2$ always yields -1 and results in the state $A(\rho_1)$ (either e_2 or e_3), if made. The measurement at $t = 3$ yields -1 if the measurement at $t = 2$ was carried out previously, else it yields $+1$. The measurement at $t = 4$ results in -1 if only one measurement was made before.*

Therefore, starting with e_1, we can now violate the Tsirelson bound for the 4-correlator Leggett-Garg inequality even more and even saturate the logical bound:

$$C_{14} + C_{12} + C_{34} - C_{23} = -4 \quad \text{(density cube } \hat{T}) \tag{4.23}$$

In principle $\hat{T}$ can be understood just as T (see the interpretation in section 4.4.3); in particular it also cannot violate the quantum bound in the spatial case. The difference is "more dependent" on the state it is applied to, and it violates the quantum signalling condition (theorem 4.9), reaching $S_+ = S_- = 1$. We can thus understand the signalling bound as a necessary, but not sufficient condition for quantum behaviour.

property but not a physical requirement. Positivity is still guaranteed for the subset of density cubes consisting of e_1, e_2, e_3 and ρ_1, ρ_2, ρ_3

5. Conclusion

I have shown that higher order interference theories, such as the *density cube* theory, which account, additionally to second order interference (as in quantum mechanics), for n-th (and n-th order only) order interference cannot both (1) recover quantum mechanics as a special case and (2) predict experimental results different from quantum mechanics. I therefore concluded that this class of theories was not a good candidate for a generalization of quantum theory.

Examining the T-transformation of density cubes, which permits a violation of the quantum (Tsirelson) bound of a temporal inequality, I have shown why the most natural generalization of the quantum part is not completely positive (assuming composite systems are obtained using the tensor product), conjectured why no violation of the quantum bound was found in the spatial case and presented a modified version $\hat{T}$, which violates the quantum bound maximally.

It remains an open question if higher order interference theories allowing second, n-th order interference, as well as other orders of interference between 2 and n could provide a generalization of quantum theory. Another open field of investigation is the four-level system as described by the density cube theory. It would be of interest to examine if it is possible to construct a transformation for a four-level system density cube, accounting for violation of the quantum temporal bound as well as the quantum spatial bound.

Another open question is if there is another way to describe composite systems of density cubes, i.e. if composite systems have a Schmidt decomposition in the density cube formalism.

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A. Deutschsprachige Zusammenfassung

In dieser Masterarbeit wurden Theorien untersucht, die neben Interferenz zweiter Ordnung (wie in der Quantenmechanik, wo diese Interferenz durch Einträge einer Dichtematrix aufgefasst werden können) auch Interferenzterme höherer Ordnung erlauben. Die Motivation dafür lieferte die Theorie der *density cubes*, die von Dakić, Paterek und Brukner [13] ausgearbeitet wurde und es erlaubt, Interferenz dritter Ordnung zu beschreiben.

Innerhalb der *density cube* Theorie sind Transformationen möglich, die in der Quantenmechanik verboten wären. Eine Beispiel für eine solche Transformation (T) erlaubt es, die quantenmechanische Grenze (*Tsirelson-Schranke*) für das zeitliche Äquivalent der CHSH-Ungleichung zu verletzen.

Ich habe gezeigt, dass die *density cube* Theorie und allgemein alle Theorien, die zusätzlich zur Interferenz zweiter Ordnung noch Interferenz n-ter Ordnung ermöglichen, nicht als Verallgemeinerung der Quantenmechanik fungieren können, weil sie nicht zugleich (1) die Quantenmechanik als Spezialfall erklären und (2) einen von ihr unterschiedlichen empirischen Gehalt haben können. Schließlich habe ich das Verhältnis zwischen Verletzung der zeitlichen Tsirelson-Schranke (im CHSH-Szenario) und der Menge an Information, die maximal zwischen zwei Zeitpunkten ausgetauscht wird, untersucht und eine neue Transformation $\hat{T}$, welche die Tsirelson-Schranke maximal verletzt, präsentiert.

B. Danksagung

Ich möchte mich bei allen bedanken, die mich im Studium unterstützt haben, allen voran Časlav Brukner für die Betreuung der Masterarbeit. Ganz besonderer Dank gebührt meinen Eltern, die mir unentwegt Beistand gewährt haben.

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