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# L'ensemble des corrélations quantiques : inégalités de Bell, caractérisation "boîte noire" et géométrie convexe

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# The set of quantum correlations: Bell inequalities, Self-testing and Convex geometry

*L'ensemble des corrélations quantiques:  
Inégalités de Bell, Caractérisation "boîte noire" et  
Géométrie convexe*

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**Thèse soutenue à Paris-Saclay, le 30 août 2024, par**

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**Title:** The set of quantum correlations: Bell inequalities, Self-testing and Convex geometry

**Keywords:** Quantum information, Quantum correlations, Bell inequalities, Self-testing, Convex geometry

**Abstract:** One of the most puzzling facts about quantum theory is that it predicts nonlocal behaviors of nature. This naturally leads to ask whether this property is just an artifact of the theory, or if such observations could actually be made. Answering such question led John S. Bell to develop a framework allowing for the study of arbitrary theories solely based on the statistics they predict. As such, quantum based predictions were utilized to build experiments disqualifying any local theory of nature.

Conversely, studying the statistics obtainable in such experiments, as well as the set formed by all quantum statistics, has been shown to capture some of quantum theory's core properties. However, only partial descriptions of this set have been provided until now. In this thesis, we delve into the world of this quantum set, studying its geometry through the lens of self-testing, a method that allows to infer the underlying physics of a quantum experiment when specific statistics are achieved.

**Titre :** L'ensemble des corrélations quantiques: Inégalités de Bell, Caractérisation "boîte noire" et Géométrie convexe

**Mots clés:** Information quantique, Corrélations quantiques, Inégalités de Bell, Certification "boîte noire", Géométrie convexe

**Résumé :** L'un des faits les plus déroutants de la théorie quantique est qu'elle prédit des comportements non locaux de la nature. Cela conduit naturellement à se demander si cette propriété n'est qu'un artéfact de la théorie, ou si de telles observations peuvent réellement être faites. La réponse à cette question a conduit John S. Bell à développer un cadre permettant d'étudier des théories arbitraires uniquement sur la base des statistiques qu'elles prédisent. Ainsi, les prédictions quantiques ont été utilisées pour construire des expériences disqualifiant toute théorie locale de la nature. Inversement, il a été démontré que l'étude des statis-

tiques obtenues lors de ces expériences, ainsi que de l'ensemble de toutes les statistiques quantiques, permettrait de saisir certaines des propriétés fondamentales de la théorie quantique. Cependant, seules des descriptions partielles de cet ensemble ont été fournies jusqu'à présent. Dans cette thèse, nous nous plongeons dans le monde de cet ensemble de corrélations quantique, en étudiant sa géométrie à travers le *self-testing*, une méthode qui permet de déduire la physique sous-jacente d'une expérience quantique lorsque des statistiques spécifiques sont atteintes.

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# Synthèse en français

## Contexte et motivations

L'un des aspects les plus fascinants de la théorie quantique est que l'existence d'intrication entre particules prédit des corrélations qui ne peuvent pas être expliquées par un modèle local impliquant des variables cachées. Cette propriété frappante, souvent appelée non-localité de Bell [15], a d'abord été observée comme un artefact des outils mathématiques utilisés pour décrire la mécanique quantique et en particulier la fonction d'onde [1].

À la suite des travaux fondamentaux de John S. Bell [5], il a ensuite été proposé un cadre pour tester le comportement de la nature et la possibilité qu'elle soit décrite par un modèle local. L'idée d'une telle expérience de Bell est d'examiner la distribution de probabilité des résultats réalisables par un certain nombre de parties, compte tenu de certains choix aléatoires d'entrées. En fonction de la théorie sous-jacente décrivant une telle expérience, on s'attend à pouvoir observer certaines distributions, tandis que d'autres distributions sont impossibles à réaliser. Cette idée peut être traduite dans un protocole expérimental en répétant des essais identiques, où dans chacun d'eux un vérificateur alimente les dispositifs non fiables testés avec des entrées de son choix, et enregistre les résultats obtenus. À la fin, le vérificateur est en mesure d'effectuer une analyse statistique des données pour observer une certaine distribution. Par exemple, l'analyse des distributions observables dans une expérience de Bell donnée prédit que la valeur maximale d'une fonction linéaire unique de la distribution de probabilité, appelée expression de Bell CHSH, permet de faire la distinction entre ce que toutes les théories locales peuvent réaliser et ce que la théorie quantique prédit [9]. Les expérimentateurs ont donc mis tout leur cœur à utiliser la mécanique quantique et ses prédictions pour observer des distributions incompatibles avec un modèle local [6] et ont maintenant réussi à exclure ces descriptions de la nature de manière indéniable [7].

Une chose importante à souligner à propos de ces résultats est qu'ils ne dépendent pas de la validité de la théorie quantique : une expérience de Bell ne valide pas une théorie quantique, elle ne fait qu'écartier toutes les théories qui n'impliquent que des mesures locales. En pratique, cependant, les démonstrations expérimentales reposent sur les hypothèses que les entrées sont indépendantes et que les résultats de chaque partie ne peuvent dépendre des entrées des autres (en pratique, cela peut être assuré par une séparation *space-like* et l'hypothèse que l'information ne peut pas voyager plus vite que la lumière). Les théories qui vérifient ce dernier principe sont appelées *non-signaling* et comprennent la formulation moderne de la mécanique quantique. Toute conclusion tirée d'une expérience de Bell inclut donc une connaissance *a priori* de ce qui est appelé local et est supposé être *non-signaling*. Ces concepts correspondent à des principes physiques indépendants du formalisme considéré, contrairement à la théorie quantique.

L'un des principaux obstacles à la recherche d'un tel principe sous-jacent à la théorie quantique pourrait être le fait que nous ne savons toujours pas exactement quelles distributions, selon cette même théorie, peuvent être obtenue dans une expérience de Bell. L'ensemble de ces distributions, appelé ensemble quantique, doit encore être caractérisé : en effet, si la théorie prédit des distribu-

tions à observer, savoir si une distribution observée peut être prédite par la théorie est une question hautement non triviale. Cependant, des contributions importantes comme celle de Tsirelson [11] ont montré qu'il était possible de considérer l'ensemble quantique comme un ensemble convexe et donc de l'étudier d'un point de vue géométrique : on peut étudier sa topologie, décrire ses points extrémaux ou même trouver l'"équivalent quantique" des inégalités de Bell, ce qui permet de distinguer les comportements quantiques des comportements non quantiques. Les expériences de type Bell ont donc été étudiées pour leur capacité à distinguer entre différents formalismes quantiques : il a par exemple été démontré que la théorie quantique réelle prédit un ensemble de distributions strictement plus petit que la théorie quantique complexe dans les approches basées sur les réseaux [12].

L'un des résultats les plus marquants pour décrire l'ensemble quantique a été la construction d'une hiérarchie de programmation semi-définie (SDP) par Navascués, Pironio et Acín (NPA), offrant un outil pour aborder cette question en termes de famille d'ensembles de distribution convergeant vers l'ensemble quantique depuis l'extérieur [13]. Cependant, cette construction implique des variables supplémentaires dont les valeurs sont a priori inconnues, et le niveau de la hiérarchie qui doit être atteint pour fournir une réponse définitive pourrait être supposé infini.

D'autres travaux ont mis en lumière des liens inattendus entre les expériences de Bell et la théorie quantique. Les violations des inégalités de Bell donnent des indications sur la description formelle des dispositifs physiques, comme la non-séparabilité de l'état. Les violations maximales de certaines inégalités de Bell sont même réalisées de manière unique par des états et des mesures spécifiques du formalisme, jusqu'à certains degrés de liberté locaux. Cette propriété frappante, appelée *self-testing* [14], joue un rôle important dans de nombreux protocoles d'information quantique. En effet, cette méthode ne requiert aucune hypothèse sur le fonctionnement interne des appareils de mesures et des sources utilisés, et ouvre donc la porte à une gamme de protocoles appelés *device-independent*, ou protocoles "boîte-noire". Cette approche fournit également un aperçu de l'ensemble quantique lui-même, car le *self-test* identifie des distributions quantiques extrêmes. Bien que le *self-testing* ait été principalement observé en fonction de la violation maximale de certaines inégalités de Bell, d'autres résultats sont basés sur la connaissance de la distribution de probabilité complète. L'approche du *self-testing* s'est avérée capable d'identifier de manière unique non seulement des états maximalement intriqués mais aussi des états partiellement intriqués, se trouvant dans des espaces de Hilbert de dimensions arbitraires.

Cette thèse vise à mieux comprendre la relation entre les corrélations quantiques, les inégalités de Bell et le *self-testing*. Nos motivations sont doubles. D'une part, comprendre ce que la théorie quantique peut réaliser dans les expériences de Bell est de la plus haute importance d'un point de vue fondamental. D'autre part, les corrélations quantiques dans les expériences de type Bell et les tests automatiques se sont révélés très prometteurs dans les protocoles de traitement de l'information [15]. Des cas d'utilisation ont été trouvés par la mise en œuvre de systèmes de certification, par exemple dans les communications sécurisées ou l'informatique quantique déléguée [16, 17]. Avec le développement rapide de ces technologies, une meilleure compréhension des principes sous-jacents est nécessaire pour améliorer la portée, l'efficacité et la praticité de ces mises en œuvre. De manière plus frappante, de nombreux protocoles utilisant le *self-testing* reposent en fait sur l'hypothèse que la physique à l'intérieur de l'expérience est effectivement décrite par la théorie quantique. Il est donc d'autant plus important de certifier que la théorie quantique est en fait une description complète

et qu'aucune autre physique plus grande que la physique quantique ne peut briser les preuves de sécurité.

## Organisation du manuscrit

Le premier chapitre de la thèse présente les concepts clés qui sous-tendent la majeure partie du manuscrit. En particulier, il donne un aperçu clair des notations qui seront utilisées et rappelle les définitions, notamment, des corrélations quantiques, des inégalités de Bell et du *self-testing*. Il introduit également quelques notions de géométrie convexe avec lesquelles certains lecteurs pourraient être moins familiers.

Le deuxième chapitre présente une expérience de Bell menée à Zurich sur deux qubits supraconducteurs à une distance de 30 mètres l'un de l'autre, voir Fig. 1. Cette collaboration avec une équipe expérimentale montre comment les concepts théoriques présentés dans le premier chapitre sont mis en œuvre dans la pratique. Elle met également en évidence les défis pratiques à relever pour réaliser une certification d'états et de mesures quantiques de manière indépendante des appareils utilisés ("boîte-noire"). Cette expérience constitue la première fois qu'un *self-testing* robuste aux erreurs expérimentales est conduit de manière complète sur l'état et sur les mesures utilisés, et ce en prenant en compte les effets dus aux statistiques finies. Cet apport ouvre la voie à l'utilisation du *self-testing* comme protocole de certification.

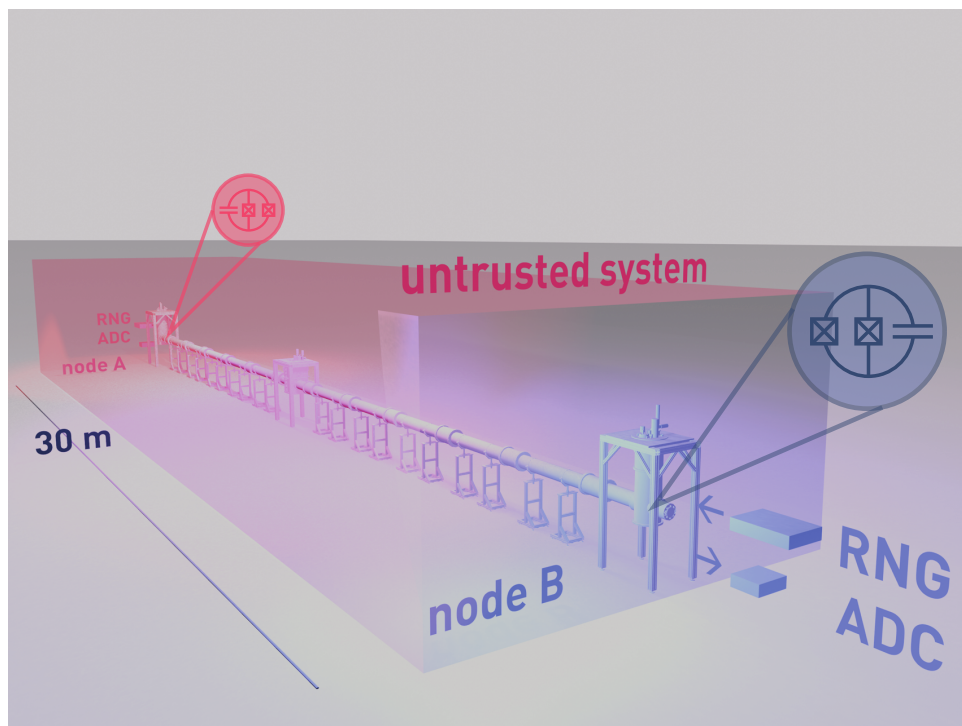


Figure 1: Schéma du montage expérimental mis en place par l'équipe de recherche à l'ETH à Zurich. Les deux qubits supraconducteurs, situés aux nœuds A et B, sont séparés par un tunnel de 30m de long, refroidi à 15mK, servant à distribuer l'intrication.



Le troisième chapitre se concentre sur la tâche consistant à dériver des expressions de Bell adaptées à la caractérisation de l'état d'une cible et/ou des mesures d'une cible. Le *self-testing* étant la pierre angulaire des protocoles "boîte-noire", il apparaît nécessaire de pouvoir caractériser les ressources les plus adaptées à chaque protocole. Pour ce faire, nous présentons une méthode qui utilise la somme formelle des carrés (SOS), ainsi que plusieurs exemples d'application. Nous utilisons cette méthode pour dériver de nouvelles inégalités adaptées à l'état à deux qubits maximalesment intriqués et de nouveaux *self-tests* pour l'état à deux qubits partiellement intriqués, impliquant des paramètres de mesure plus larges que les résultats précédemment connus. Notons que la méthode que nous présentons fournit des conditions nécessaires et asymptotiquement suffisantes.

Le quatrième chapitre complète le précédent en présentant comment trouver toutes les expressions de Bell qui sont maximisées par une réalisation donnée. Si l'objectif présenté apparaît comme théorique, il n'en reste pas moins d'intérêt pratique : à protocole (et donc réalisation) donné se pose la question du meilleur témoin de certification pouvant être utilisé. Le choix de ce dernier peut dépendre des bruits ou des contraintes expérimentales propres à chaque expérience. L'approche novatrice que nous adoptons dans ce chapitre repose sur des outils de géométrie convexe et plus particulièrement sur la notion de dualité des ensembles convexes. Après avoir présenté cette approche générale, nous nous concentrons sur l'étude du point de Tsirelson, distribution ayant joué un rôle historique dans le domaine de l'information quantique, notamment comme étant le seul qui maximise l'inégalité CHSH. Nos résultats s'articulent autour de deux axes : du point de vue du *self-testing*, nous montrons que ce point peut être caractérisé avec une famille d'inégalités à deux paramètres ; du point de vue géométrique, notre travail apporte un éclairage nouveau sur la géométrie de l'ensemble quantique puisque nous prouvons que ce point est anguleux et, dans une projection donnée, se trouve au sommet d'une pyramide à base octogonale, voir Fig. 2.

Le cinquième et dernier chapitre fournit la première description analytique de l'ensemble quantique dans le scénario de Bell avec deux parties, deux entrées et deux réponses possibles. Cette description est fournie par une paramétrisation complète des points extrêmes de l'ensemble quantique, avec une interprétation géométrique claire. Nous montrons en particulier que tous les points extrêmes dans ce scénario fournissent un *self-testing* d'une réalisation réelle impliquant un état de deux qubit et des mesures dans le plan  $(\sigma_z, \sigma_x)$  satisfaisant une condition d'alternance. Ceci fournit tous les *self-tests* pour ce scénario. Notre travail repose sur la découverte d'une nouvelle transformation non linéaire basée sur le *steering*, qui permet d'exprimer une réalisation impliquant un état partiellement intriqué en termes de quatre sous-réalisations impliquant un état maximalesment intriqué. Cette transformation, ainsi que les éléments constituant les preuves des résultats, nous semblent fournir une base solide pour décrire l'ensemble quantique dans des scénarios de Bell plus complexes.

De manière générale, cette thèse explore en profondeur la relation entre corrélations quantiques et *self-testing* en scénario de Bell. En envisageant le développement de nouvelles applications prometteuses à travers des dispositifs innovants et des méthodes de communication avancées, et donc la croissance rapide des technologies basées sur la mécanique quantique, il devient essentiel de certifier leur bon fonctionnement. Dans cette optique, le *self-testing* apparaît comme un outil de premier choix. Bien que des progrès significatifs aient été accomplis, beaucoup de questions théoriques restent ouvertes, notamment concernant la description géométrique complète de l'ensemble quantique et sa relation avec son dual. L'étude des corrélations quantiques dans des scénarios élargis et

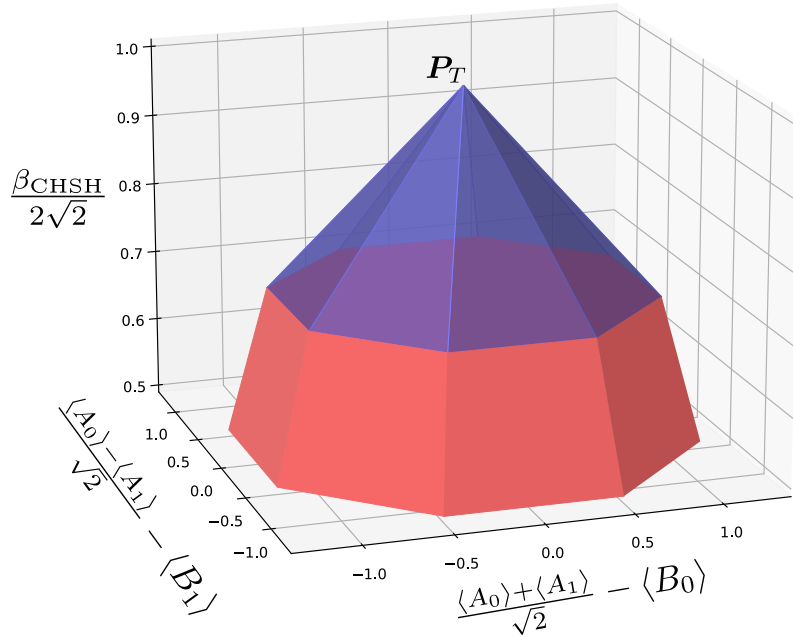


Figure 2: Projection tri-dimensionnelle de l'ensemble des corrélations locales (en rouge) et de l'ensemble quantique (en rouge et bleu) pour un scénario de Bell avec deux parties ayant chacun deux entrées et deux réponses possibles. Dans cette projection, le point de Tsirelson,  $P_T$ , se trouve au sommet d'une pyramide à base octogonale.

l'application de ces résultats à des protocoles quantiques plus robustes sont des pistes importantes pour les travaux futurs. En somme, cette thèse apporte des outils mathématiques et des idées novatrices pour progresser dans la description de ce que la théorie quantique peut accomplir dans les scénarios de type Bell, et propose des résultats qui pourront non seulement enrichir la compréhension fondamentale de la théorie quantique, mais aussi favoriser le développement d'applications pratiques, notamment dans les domaines de la certification et de la sécurité quantique.



# List of publications

This thesis is based on the following contributions.

1. *Custom Bell inequalities from formal sums of squares*,  
Victor Barizien, Pavel Sekatski, Jean-Daniel Bancal,  
Quantum 8, 1333 (2024).
2. *Extremal Tsirelson inequalities*,  
Victor Barizien, Jean-Daniel Bancal,  
Phys. Rev. Lett. 133, 010201 (2024).
3. *Complete Self-Testing of a Remote Superconducting Qubits System*,  
Simon Storz, Anatoly Kulikov, Josua D. Schär, Victor Barizien, Xavier Valcarce, Florence Berterot-  
tière, Nicolas Sangouard, Jean-Daniel Bancal, and Andreas Wallraff,  
*pre-print*, arXiv:2408.01299
4. *Quantum statistics in the minimal scenario*,  
Victor Barizien, Jean-Daniel Bancal,  
*pre-print*, arXiv:2406.09350

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# Introduction

## Background and motivations

A theoretical physicist is someone who specializes in mathematical modeling of physical systems to rationalize our understanding of natural phenomena. This modeling can be a two-way road: on one hand, it can be driven by an observed, yet unexplained, phenomenon, for which a new theory is needed; on the other hand, a given theory can predict new phenomena, yet to be observed. While the first way could be extremely challenging, the latter may just simply be impossible. Indeed, predictions from a purely mathematical theory may not have any physicality: the theory and the physics it describes are two very distinct, yet indivisible, objects, as perfectly summarized by Einstein, Podolsky and Rosen [1]:

*"Any physical consideration of a physical theory must take into account the distinction between the objective reality, which is independent of any theory, and the physical concepts with which the theory operates."*

When these two don't match, a question arises: should the theory be modified to only account for the objective reality, or should one keep pushing harder to observe the physical concepts it predicts?

Quantum theory has been, from its faltering steps up to nowadays, an amazing example of this dilemma. Max Planck himself, a pioneer of the field, thought of the quanta (from which the name of the theory comes from), introduced to explain black-body radiations, as a purely formal assumption. He wrote in a letter in 1931 [2]:

*"I really did not give it much thought except that no matter what the cost, I must bring about a positive result."*

Quantum theory was born: physicists allowed themselves for heuristic mathematical corrections of existing theories to explain physical observations with unprecedented precision.

With the development of such models to express various phenomena, such as particle/wave duality of light or diamagnetism, soon came the need for a unifying theory. With it came a load of new mathematical objects: particles' states took the form of *wave functions* over Hilbert spaces, on which *measurements* could be performed. Interestingly, at a 30 years interval, the same Einstein who proved that Planck's quanta had an objective reality, disbelieved some of the physical concepts introduced by this new formalism. Indeed, this



theory predicted that measurements performed on the wave function could instantaneously modify the state of a particle across the whole space, thus leading to a highly nonlocal operation. Again came the intrinsic dilemma of theoretical physics: does the wave function and the measurement process have no physicality, or can we observe nonlocal phenomena matching the theory's predictions?

These questions raised over the years a debate on whether quantum theory is ontic or epistemic, i.e. whether every element of the theory describes a physical reality or only observers' beliefs about the physical state. Regarding the wave function, Harrigan and Spekkens proposed a mathematical framework for the debate [3], which allowed to prove, under reasonable independence assumptions, that the wave function of any quantum theory can be seen as ontic [4]. Then again, as these results rely on a given mathematical formulation of the underlying problem, they could be prone to criticism.

Regarding the measurement process, its nature is still under vivid debate, but its nonlocality has been treated as an independent line of work. Following the seminal work of John S. Bell [5], it has been later proposed a framework to test the behavior of nature and the possibility that it could be described by a local model. The idea of such a *Bell experiment* is to consider the probability distribution of outputs achievable by a number of parties, given some random choices of inputs. Depending on the underlying theory to describe such an experiment, one expects to be able to observe some distributions, while other distributions are impossible to realize. This idea can be translated into an experimental protocol by repeating identical trials, where in each of them a verifier feeds the untrusted devices under test with inputs of his choice, and records the answered outcomes. In the end, the verifier is able to perform a statistical analysis of the data to observe some distribution. Experimentalists have therefore put their hearts to use quantum mechanics and its prediction to observe distribution incompatible with a local model [6] and have now managed to rule out these descriptions of nature in an undeniable fashion [7].

One important thing to highlight about these results is that they do not depend on the validity of quantum theory. Then again, Bell experiments were first introduced for the capacity to distinguish between local and nonlocal behaviors and have *a priori* nothing to do with quantum theory, as Froissart perfectly pointed in 1981 [8]:

*"Data violating Bell's inequalities contradict all locally causal theories, but they do not either prove or disprove quantum mechanics".*

In practice, however, experimental demonstrations rely on the assumptions that inputs are independent and that information cannot travel faster than light. Theories verifying this latter principle are called non-signaling and include the modern formulation of quantum mechanics. Any conclusion drawn

from a Bell-experiment thus includes an *a priori* knowledge of what is called local and is assumed non-signaling. These are however easier concepts to grasp as they correspond to physical principles independent of the formalism. One of the most convincing line of research to argue of quantum theory as complete has thus been to find a physical principle sufficient to match the predictions of the quantum formalism. For example, Bell experiments predict that the maximal value of a single linear function of the probability distribution, called the CHSH Bell inequality [9], allows distinguishing between what all local and non-signaling theories can achieve. Quantum theory however predicts that one can obtain a maximal value strictly between these two bounds. A convincing refinement of the non-signaling principle, called information causality<sup>1</sup>, has been proven to be sufficient to match the upper bound of quantum theory [10]. Unfortunately, this principle has been found wanting, as it allows for other distributions the formalism doesn't predict.

One of the main obstacle for the search of this underlying principle might be the fact that we still actually don't know exactly what distribution quantum theory predicts to be achievable in a Bell experiment. The ensemble of such distributions, referred to as the quantum set, is yet to be characterized: indeed, if the theory predicts distributions to be observed, it is a highly non-trivial question to know whether an observed distribution can be predicted by the theory. However, important contributions such as Tsirelson's [11] showed that it was possible to consider the quantum set as a convex ensemble and thus study it from a geometrical perspective: one can study its topology, describe its extremal points or even find the "quantum equivalent" of Bell inequalities<sup>2</sup>, allowing to distinguish between quantum and non-quantum behaviors. Bell-like experiments have therefore been studied for their ability to distinguish between different quantum formalisms: real quantum theory has been shown to predict a strictly smaller set of distributions than complex quantum theory in network-based approaches [12].

One of the most prominent results to describe the quantum set has been the construction of a hierarchy of semi-definite programming by Navascués, Pironio and Acín (NPA) offering a tool to tackle this question in terms of a family of distribution sets converging to the quantum set from the outside [13]. This hierarchy is now a central tool of quantum information science, with an impact reaching optimization theory. However, this construction involves additional variables whose values are a priori unknown, and the level of the hier-

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<sup>1</sup>Formulated as a principle, information causality states: "the information gain that Bob can reach about a previously unknown to him data set of Alice, by using all his local resources and  $m$  classical bits communicated by Alice, is at most  $m$  bits" [10, p. 1101]

<sup>2</sup>Just like Bell's seminal contribution gave his name to Bell inequalities, one could call there quantum equivalent Tsirelson inequalities, in the memory of Tsirelson's seminal work.

archy which must be reached in order to provide a definitive answer could be supposedly infinite. It can still be used efficiently at a finite level of relaxation to ensure that given distributions are not predicted by quantum theory.

Other lines of work have shed light on unexpected links between Bell experiments and quantum theory. Violations of Bell inequalities provide insights on the formal description of the physical devices, such as non-separability of the state. Maximal violations of some Bell inequalities are even uniquely achieved by specific states and measurements of the formalism, up to some local degrees of freedom. This striking property, called *self-testing* [14], plays an important role in many quantum information protocols, but also provides an insight on the quantum set itself as self-testing identifies extremal quantum distributions. Even though self-testing was mainly observed according to the maximal violation of some Bell inequalities, other results are based on the knowledge of the full probability distribution. This method has been shown to be able to uniquely identify not only maximally entangled states but also partially entangled ones, lying in Hilbert spaces of arbitrary dimensions.

This thesis aims to better understand the relationship between quantum correlations, Bell inequalities and self-testing. Our motivations are twofold. On one hand, understanding what quantum theory can achieve in Bell experiments is of foremost importance from a fundamental point of view: testing the completeness of quantum theory requires to better understand what is quantum and what isn't. On the other, quantum correlations in Bell-like experiments and self-testing have been proven to be very promising in information processing protocols [15]. Use cases were found through the implementation of certification schemes, for example in secure communications or delegated quantum computing [16, 17]. With the quick development of such technologies, a better understanding of the underlying principles is necessary to enhance the range, the efficiency and the practicality of such implementations. More strikingly, many protocols utilizing self-testing actually rely on the assumption that the physics inside the experiment is indeed described by quantum theory. This makes it even more important to certify that quantum theory is actually a complete description and that no other larger-than-quantum physics could break the security proofs.

## Organization of the manuscript

The first chapter of the thesis introduces the key concepts that underline most of the manuscript. In particular, it gives a clear overview of the notations that will be used and recalls the definitions of, most notably, quantum correlations, Bell inequalities and self-testing. It also introduces some notions of convex geometry with which some reader might be less familiar with.

The second chapter showcases a Bell experiment that was conducted in Zurich on two superconducting qubits at a distance of 30 meters from one another. This collaboration with an experimental team sheds light on how the theoretical concepts introduced in the first chapter are implemented in practice. It also highlights the practical challenges to perform device-independent certification.

The third chapter focuses on the task of deriving Bell expressions that are suited for the characterization of a target state and/or target measurements. To do so, we present a method that uses formal Sum of Squares, along with several examples. We use this method to derive new inequalities tailored to the maximally entangled two qutrit state and new self-tests for the partially entangled two qubit state, involving broader measurements parameters than previously known results. Note that the method we present provides necessary conditions for the task and is asymptotically complete.

The fourth chapter complements the previous one as it presents how to find all Bell expressions that are maximized by a given realization. After showcasing our general approach, we focus on the study of the Tsirelson point, the only one maximizing the CHSH inequality. Our results are divided along two lines: from a self-testing point of view, we show that this point can be self-tested with a two parameter family of inequalities; from a geometrical point of view, our work provides fresh insight on the geometry of the quantum set as we prove that this point is angular and, in a given projection, lies on top of an octagonal based pyramid.

The fifth and final chapter provides the first analytical description of the quantum set in the Bell scenario with two parties, two inputs and two outputs. This description is provided by a full parameterization of the extremal point of the quantum set, with a clear geometrical interpretation. Our work relies on the discovery of a new non-linear transformation based on steering, that allows expressing a realization involving a partially entangled states in terms of four sub-realizations involving a maximally entangled one. This provides all the self-tests for this scenario.



# I – Definitions, Key concepts and Notations

## I.1 - Bell nonlocality

### I.1.1 . Bell experiment

In his seminal work, John S. Bell introduced a framework to put to a test the local nature of physics [18]. The idea is to take two parties (that we like to call Alice and Bob) and put them in two labs. They are then going to play a game where at each round they are going to be asked a random question, say  $x = 0, 1$  for Alice and  $y = 0, 1$  for Bob, and will have to give a binary answer,  $a \in \{-1, +1\}$  for Alice and  $b \in \{-1, +1\}$  for Bob. If you make them play a very large number of rounds and record for each round the inputs that were received, and the outputs that were given, you will be able to infer the probability to observe specific pairs of answers with respect to the questions asked. This set of 16 probabilities can be encoded into a vector

$$\vec{P} = \{p(\mathbf{ab}|xy)\}_{\mathbf{ab}xy} \in \mathbb{R}^{16} \quad (\text{I.1})$$

Note that we did not assume anything about the link that could exist between Alice and Bob, whether during or before the experiment is played, neither on how they decide on their answers. For one thing, Alice and Bob could be on the phone during the experiment! Restricting what Alice and Bob can do, i.e. imposing constraints on the way the experiment is played, the devices they have access to or the laws of physics that rule this world, allows for different probabilities  $\vec{P}$  to be observed.

The only thing that one can say about such probabilities is that they are observed in the physical realm and as such they must be valid probability distribution, i.e. verify:

$$\text{positivities: } \forall \mathbf{a}, \mathbf{b}, x, y, p(\mathbf{ab}|xy) \geq 0, \quad (\text{I.2a})$$

$$\text{normalization: } \forall x, y, \sum_{\mathbf{a}, \mathbf{b}} p(\mathbf{ab}|xy) = 1. \quad (\text{I.2b})$$

Even though we introduced the idea of Bell experiment for only two parties each having two possible inputs and outputs, the idea can be generalized to an arbitrary number of each of these. Each form a different scenario for which it will be possible to infer some probability vector that can be achieved or not among specific assumptions. For the rest of the manuscript, when dealing with such scenarios, we will denote them as  $(n, m, k)$  where  $n$  is the number of parties,  $m$  and  $k$  are respectively the number of inputs and outputs

for each party. If nothing is specified, consider that we are in the scenario presented before, referred to as the CHSH scenario.

### I.1.2 . The non-signaling set

A first constraint that can be applied on the two parties is that they are not able to communicate their inputs with one another. One way to impose this information principle is to assume that inputs have no physical reality before they are given to the parties and to trust that the laws of physics do abide to the principle of special relativity, which states that information cannot travel faster than the speed of light  $c$ . As such, if one puts Alice and Bob sufficiently far apart, at distance  $d$ , and ask them to answer within a short enough time frame  $t < d/c$ , one can ensure that the outcome  $a$  of Alice does not depend on the input  $y$  of Bob, and vice versa.

Such an assumption implies operational restrictions on the probabilities  $\vec{P}$  that can be observed. Mathematically speaking, it means that the marginals probabilities of each party are well-defined:

$$\forall a, x, p(a|x) := \sum_b p(ab|xy) \text{ doesn't depend on } y, \quad (I.3a)$$

$$\forall b, y, p(b|y) := \sum_a p(ab|xy) \text{ doesn't depend on } x. \quad (I.3b)$$

When probabilities obey this principle and Eq. (I.2), we say that they are non-signaling. The set of all such probability vectors, denoted  $\mathcal{N}$  in the following, is a first physical set of interest as it encodes a fundamental principle.

Note that when a probability vector is non-signaling, it can be convenient to introduce new quantities, called correlators, defined in the following way:

$$\text{correlations: } \langle A_x B_y \rangle = \sum_{ab} ab p(ab|xy), \quad (I.4a)$$

$$\text{marginals: } \langle A_x \rangle = \sum_a a p(a|x), \quad (I.4b)$$

$$\langle B_y \rangle = \sum_b b p(b|y). \quad (I.4c)$$

Non-signaling and normalization conditions allows for a one to one identification between correlators and probabilities. This change of variable allows to study a vector of correlators that is embedded in  $\mathbb{R}^8$  only. The positivity constraints can be translated to inequalities on the correlators as:

$$\forall a, b, 1 + a\langle A_x \rangle + b\langle B_y \rangle + ab\langle A_x B_y \rangle \geq 0. \quad (I.5)$$

In the following, we will sometimes use a representation of these correlators in tables, defined by

$$\vec{P} = \begin{array}{c|cc} & \langle B_0 \rangle & \langle B_1 \rangle \\ \hline \langle A_0 \rangle & \langle A_0 B_0 \rangle & \langle A_0 B_1 \rangle \\ \hline \langle A_1 \rangle & \langle A_1 B_0 \rangle & \langle A_1 B_1 \rangle \end{array}. \quad (I.6)$$

### I.1.3 . The local set

One thing that Alice and Bob could do before playing the game is that they would meet up and craft a strategy on how to produce the answers. It could also be that their labs share a similar painting encoding for a secret message. To account for all those past events that could have happened before the experiment between the labs of Alice and Bob, one can consider a variable  $\lambda$  that is shared between the two. The physical hypothesis of *locality*, which state that the physical measurements are local procedures, ensures that the answers given by each party only depend on their input and their past, and not on the answer given by the other player. The probabilities should thus factorize in the following way:

$$p(\mathbf{ab}|xy, \lambda) = p(\mathbf{a}|x, \lambda)p(\mathbf{b}|y, \lambda). \quad (I.7)$$

where  $p(\mathbf{a}|x, \lambda)$  and  $p(\mathbf{b}|y, \lambda)$  are themselves valid probability distributions. To take into account the fact that the common past of Alice and Bob may not be deterministic, one can consider that  $\lambda$  is a continuous probability distribution. Locality therefore allows for any probability vector verifying

$$p(\mathbf{ab}|xy) = \int_{\lambda} p(\mathbf{a}|x, \lambda)p(\mathbf{b}|y, \lambda)p(\lambda)d\lambda \quad (I.8)$$

and the set of all such vectors is called the local set, denoted  $\mathcal{L}$ . Conversely, any vector  $\vec{P} \in \mathbb{R}^8$  for which Eq. (I.8) does not hold is called nonlocal. Note that every vector in  $\mathcal{L}$  is also in  $\mathcal{N}$ .

### I.1.4 . The quantum set

If Alice and Bob were to be two physicists, they might have heard about quantum mechanics and the notion of entanglement. This striking property implies that measurements performed on a physical state can alter its state instantaneously. In particular, they could get the idea to share beforehand some entangled particles and perform measurements on it to predict their answers. The probabilities that they could obtain by doing so can be predicted by quantum mechanics and Born's rule to be:

$$p(\mathbf{ab}|xy) = \text{Tr}_{AB}((\Pi_{\mathbf{a},x} \otimes \Pi_{\mathbf{b},y})\rho_{AB}) \quad (I.9)$$

where  $\rho_{AB}$  is the density matrix of the shared state,  $\Pi_{\mathbf{b},y}$  are the local projective measurements performed by Alice and Bob respectively. As such, they verify  $\rho_{AB} \geq 0$ ,  $\text{Tr}(\rho_{AB}) = 1$ ,  $\Pi_{\mathbf{a},x}\Pi_{\mathbf{a}',x} = \delta_{\mathbf{a}\mathbf{a}'}\Pi_{\mathbf{a},x}$  and  $\sum_{\mathbf{a}} \Pi_{\mathbf{a},x} = \mathbf{1}_A$  (likewise for Bob), ensuring that the obtained probability vector is in  $\mathcal{N}$ .

One very important thing to notice is that Alice and Bob could have local Hilbert spaces of arbitrary large dimensions. Every vector of probabilities that admits local Hilbert spaces, a shared state and local measurements such that



Eq. (I.9) holds is called a quantum point. The set of all such points is the quantum set, denoted  $\mathcal{Q}$ . It is a set of physical interest, as it encodes for everything achievable within quantum theory in a Bell experiment.

Note that if they decide to share a separable state, i.e. that the density matrix can be decomposed as  $\rho_{AB} = \sum_i \lambda_i \rho_A^{(i)} \otimes \rho_B^{(i)}$  (with  $\lambda_i \geq 0$  and  $\sum_i \lambda_i = 1$ ) then, not so surprisingly, the corresponding probability vector satisfies

$$p(\text{ab}|xy) = \sum_i \lambda_i \text{Tr}_A(\Pi_{\text{a},x} \rho_A^{(i)}) \text{Tr}_B(\Pi_{\text{b},y} \rho_B^{(i)}) \quad (\text{I.10})$$

and is thus fully local. The notion of separability in quantum mechanics is thus intrinsically linked with the notion of locality.

Finally, in a scenario with only two outputs per party, it is often useful to consider the unitary operators

$$A_x = \Pi_{+,x} - \Pi_{-,x}, \quad B_y = \Pi_{+,y} - \Pi_{-,y} \quad (\text{I.11})$$

which verify  $A_x^2 = B_y^2 = 1$ . Indeed, these allow for a simpler expression of the correlators:

$$\langle A_x B_y \rangle = \text{Tr}((A_x \otimes B_y) \rho_{AB}), \quad (\text{I.12a})$$

$$\langle A_x \rangle = \text{Tr}(A_x \rho_{AB}), \quad \langle B_y \rangle = \text{Tr}(B_y \rho_{AB}). \quad (\text{I.12b})$$

In the following we will call  $(\rho, A_x, B_y)$  a *realization*. Every realization gives a well-determined correlator vector through the above equation.

### I.1.5 . Bell expressions

To distinguish between local and nonlocal correlations, Bell had the idea of computing inequalities that would be valid for all probability vectors verifying the hypothesis of local realism. These inequalities take the following form:

$$\vec{\beta} \cdot \vec{P} \leq \beta_{\mathcal{L}} \quad (\text{I.13})$$

where  $\vec{\beta} \in \mathbb{R}^{16}$ ,  $\cdot$  is the canonical scalar product of  $\mathbb{R}^{16}$  and  $\beta_{\mathcal{L}}$  is the maxima of the left-hand side for all possible vectors  $\vec{P} \in \mathcal{L}$ . As such, any probability vector  $\vec{P}$  verifying  $\vec{\beta} \cdot \vec{P} > \beta_{\mathcal{L}}$  is nonlocal: we say that it violates this Bell inequality. In what follows, we will refer to  $\vec{\beta}$  as the Bell expression underlying the inequality.

The mindful reader will have noticed that we already encountered Bell inequalities in our preliminary remarks in the form of the positivity constraints Eq. (I.2a). However, they are not particularly relevant to explore as they are verified by all non-signaling correlations. As such, no physical model that one could think of would allow for a violation of these inequalities.

One of the first and most interesting inequality that was proposed to test the local nature of physics was the CHSH inequality [9]:

$$\sum_{\text{abxy}} \text{ab}(-1)^{xy} p(\text{ab}|xy) \leq 2. \quad (\text{I.14})$$

which can be reformulated in terms of correlators as

$$\langle A_0 B_0 \rangle + \langle A_1 B_0 \rangle + \langle A_0 B_1 \rangle + \langle A_1 B_1 \rangle \leq 2. \quad (\text{I.15})$$

This inequality allows for non-trivial violations within the framework of quantum mechanics. Indeed, if Alice and Bob share a maximally entangled two qubit state

$$|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \quad (\text{I.16})$$

and perform measurements

$$A_0 = \sigma_z, \quad A_1 = \sigma_x, \quad (\text{I.17a})$$

$$B_0 = \frac{\sigma_z + \sigma_x}{2}, \quad B_1 = \frac{\sigma_z - \sigma_x}{2}, \quad (\text{I.17b})$$

they will obtain the following correlators:

$$\vec{P}_T = \begin{array}{c|c|c} & 0 & 0 \\ \hline 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \hline 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{array}. \quad (\text{I.18})$$

As such, this realization gives a Bell violation of  $2\sqrt{2}$ . One can prove that this is the maximal value for any point in  $\mathcal{Q}$ . Likewise, one can find that there exists some non-signaling correlators that give violations up to 4. As such, the CHSH expression gives rise to three different inequalities:

$$\vec{\beta}_{\text{CHSH}} \cdot \vec{P} \leq \begin{cases} 2 & \text{if } \vec{P} \in \mathcal{L}, \\ 2\sqrt{2} & \text{if } \vec{P} \in \mathcal{Q}, \\ 4 & \text{if } \vec{P} \in \mathcal{N}. \end{cases} \quad (\text{I.19})$$

The largest value that one can reach with quantum theory, here  $2\sqrt{2}$ , is called the Tsirelson bound of the Bell expression, denoted  $\beta_{\mathcal{Q}}$ . In general, one can refer to the quantum inequality  $\vec{\beta} \cdot \vec{P} \leq \beta_{\mathcal{Q}}$  as the corresponding Tsirelson inequality. Quite remarkably, note that a single Bell expression is sufficient to distinguish between the three sets of physical interest and to state that

$$\mathcal{L} \subsetneq \mathcal{Q} \subsetneq \mathcal{N}. \quad (\text{I.20})$$

### I.1.6 . Elements of Convex Geometry

Every single set we have considered so far is convex. For the non-signaling set, it is because it arises from linear constraints only and those are preserved by convexity. For the local set, we constructed it as the convex mixture, with weight  $\lambda$ , of every separable probabilities, see Eq. (I.8). Finally, for the quantum set, convexity arises from the unboundness of the local Hilbert space dimensions. Indeed, if one considers two quantum points  $\vec{P}^{(1)}, \vec{P}^{(2)}$ , admitting

two realizations  $(\rho^{(1)}, A_x^{(1)}, B_y^{(1)})$  and  $(\rho^{(2)}, A_x^{(2)}, B_y^{(2)})$  on local Hilbert space  $L(\mathcal{H}_{A(B)}^{(k)})$ , then for any  $p \in [0, 1]$

$$\rho = p\rho^{(1)} \oplus (1-p)\rho^{(2)}, \quad A_x = A_x^{(1)} \oplus A_x^{(2)}, \quad B_y = B_y^{(1)} \oplus B_y^{(2)} \quad (1.21)$$

is a valid realization on larger local Hilbert spaces  $L(\mathcal{H}_{A(B)}^{(1)} \oplus \mathcal{H}_{A(B)}^{(2)})$  whose correlation vector is  $\vec{P} = p\vec{P}^{(1)} + (1-p)\vec{P}^{(2)}$ . As such, convex geometry seems like a tool of particular interest for the study of these three sets.

One subset of remarkable points of a convex set  $\mathcal{K} \subset \mathbb{R}^n$  is the set of *extremal points*, denoted  $\text{Ext}(\mathcal{K})$ . Extremal points are ones that cannot be decomposed as convex mixture of two other distinct points, i.e.  $\vec{P} \in \mathcal{K}$  verifying

$$\forall \vec{P}_1, \vec{P}_2 \in \mathcal{K}, p \in [0, 1], \vec{P} = p\vec{P}_1 + (1-p)\vec{P}_2 \implies \vec{P}_1 = \vec{P}_2 = \vec{P}. \quad (1.22)$$

In finite dimension, convex sets are exactly the convex hull of their extremal points, i.e.  $\mathcal{K} = \text{Conv}(\text{Ext}(\mathcal{K}))$  [19, Corollary 18.5.1]. As such, the knowledge of the extremal points of a convex set is of foremost importance. For example, the non-signaling set admits 24 extremal points given by

$$\vec{P}_{a,a',b,b'}^D = \begin{array}{c|cc} & b & b' \\ \hline a & ab & ab' \\ \hline a' & a'b & a'b' \end{array}, \quad \vec{P}_{\epsilon,\alpha,\beta}^{PR} = \begin{array}{c|cc} & 0 & 0 \\ \hline 0 & \epsilon & \epsilon\alpha \\ \hline 0 & \epsilon\beta & -\epsilon\alpha\beta \end{array} \quad (1.23)$$

where  $\vec{P}_{a,a',b,b'}^D$  for  $a, a', b, b' \in \{-1, 1\}$  are called deterministic points, and  $\vec{P}_{\epsilon,\alpha,\beta}^{PR}$  for  $\epsilon, \alpha, \beta \in \{-1, 1\}$  are called PR-boxes. Note that the later don't admit any local nor quantum realization. The extremal points of the local set are also known and consist of the 16 deterministic points. As such, both  $\mathcal{L}$  and  $\mathcal{N}$  admit a finite number of extremal points and are thus *polytopes*. On the other hand,  $\mathcal{Q}$  admits an infinite number of extremal points, which makes it way harder to characterize.

Another useful tool for the study of convex sets is the notion of duality. The dual of a convex set  $\mathcal{K} \in \mathbb{R}^n$  is defined as

$$\mathcal{K}^* = \{\vec{\beta} \in \mathbb{R}^n : \forall \vec{P} \in \mathcal{K}, \vec{\beta} \cdot \vec{P} \leq 1\}. \quad (1.24)$$

In terms of nonlocality, the dual encodes the bound of every Bell expression for a given set of correlators  $\mathcal{K}$ . For example,  $\vec{\beta}_{\text{CHSH}}/2$  is an element of  $\mathcal{L}^*$  whereas only  $\vec{\beta}_{\text{CHSH}}/4$  is in  $\mathcal{N}^*$ . Note that the dual of a convex set is itself a convex set and is closely related to this original one by the dual closure  $(\mathcal{K}^*)^* = \mathcal{K}$  [19, Theorem 14.1]. Interestingly, it has been proven that the local and non-signaling polytopes are dual to one another in  $(n, 2, 2)$ -Bell scenarios, i.e.  $\mathcal{L}^* = \mathcal{N}$ , and that the subset of zero marginal quantum correlators in the CHSH scenario is its own dual [20]. However, no specific relation between the sets  $\mathcal{Q}$  and its dual  $\mathcal{Q}^*$  is known in arbitrary scenarios. Yet, as the latter

encodes the Tsirelson bound of all Bell expressions, it is equally important to describe it, as those play a key role in many quantum information protocols.

Finally, the last notion that we will introduce here is a way to distinguish between two classes of extremal points. The first class is the set of *exposed points*, which are the ones that are the unique maximizer of a given Bell expression, i.e.  $\vec{P} \in \mathcal{K}$  such that:

$$\exists \vec{\beta} \in \mathcal{K}^*, \forall \vec{P}' \in \mathcal{K}, \vec{\beta} \cdot \vec{P}' = 1 \implies \vec{P}' = \vec{P}. \quad (1.25)$$

Conversely, such expressions, sometimes called *exposing hyperplanes*, are particularly interesting because reaching their maximal value identifies a single correlator vector. On the other hand, extremal points who do not verify the above property are called *non-exposed*.

## I.2 - Self-testing

### I.2.1 . Reaching the Tsirelson bound of CHSH

We already saw that the CHSH expression is a tool of choice to study some properties of the physical system used in the experiment. For example, if one assumes that a quantum realization is performed, a CHSH value strictly larger than 2 ensures that the shared state is non-separable. An even more striking fact occurs when reaching the Tsirelson bound  $2\sqrt{2}$ .

Consider a quantum realization  $(\rho_{AB}, A_x, B_y)$  on arbitrary large local Hilbert spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$ . Suppose that the corresponding correlator vector  $\vec{P}$ , computed using Eq. (1.12), verifies  $\vec{\beta}_{\text{CHSH}} \cdot \vec{P} = 2\sqrt{2}$ . Then, one can prove the existence of local unitary maps

$$U_A \in L(\mathcal{H}_A \otimes \mathbb{C}^2), U_B \in L(\mathcal{H}_B \otimes \mathbb{C}^2), \quad (1.26)$$

which identify a system of local dimension 2 in which the performed realization corresponds exactly to the one introduced in Eqs. (1.16) and (1.17), that is:

$$(U_A \otimes U_B)(\rho_{AB} \otimes |00\rangle\langle 00|)(U_A \otimes U_B)^\dagger = \tau_{AB} \otimes |\phi^+\rangle\langle \phi^+|, \quad (1.27a)$$

$$U_A(A_0 \otimes \mathbb{1}_{\mathbb{C}^2})U_A^\dagger = \mathbb{1}_{\mathcal{H}_A} \otimes \sigma_z, \quad U_A(A_1 \otimes \mathbb{1}_{\mathbb{C}^2})U_A^\dagger = \mathbb{1}_{\mathcal{H}_A} \otimes \sigma_x, \quad (1.27b)$$

$$U_B(B_y \otimes \mathbb{1}_{\mathbb{C}^2})U_B^\dagger = \mathbb{1}_{\mathcal{H}_B} \otimes \frac{\sigma_z + (-1)^y \sigma_x}{2}. \quad (1.27c)$$

where  $\tau_{AB}$  is an unspecified state of  $\mathcal{H}_A \otimes \mathcal{H}_B$  (see [14, Section 4]). Therefore, reaching the Tsirelson bound of the CHSH expression identifies the underlying quantum realization. Furthermore, it uniquely identifies the correlators obtained by such a realization as for example

$$\begin{aligned} \text{Tr}((A_0 \otimes B_0)\rho_{AB}) &= \text{Tr}((A_0 \otimes \mathbb{1}_{\mathbb{C}^2}) \otimes (B_0 \otimes \mathbb{1}_{\mathbb{C}^2})(\rho_{AB} \otimes |00\rangle\langle 00|)) \\ &= \text{Tr}((\mathbb{1}_{\mathcal{H}_A} \otimes \mathbb{1}_{\mathcal{H}_B})\tau) \text{Tr}\left(\left(\sigma_z \otimes \frac{\sigma_z + \sigma_x}{2}\right) |\phi^+\rangle\langle \phi^+|\right) = 1 \cdot \frac{1}{\sqrt{2}}. \end{aligned} \quad (1.28)$$

Likewise, one can compute that all other correlations are given by  $\langle A_x B_y \rangle = (-1)^{xy}/\sqrt{2}$  and that marginals are  $\langle A_x \rangle = \langle B_y \rangle = 0$ . Finally, we proved that the only vector of the quantum set maximally violating the CHSH inequality is  $\vec{P}_T$  (see Eq. (I.18)). Geometrically speaking, this point, called the *Tsirelson point*, is thus an exposed extremal point of  $\mathcal{Q}$  and  $\vec{\beta}_{\text{CHSH}}/2\sqrt{2}$  is an exposing functional of this point.

### I.2.2. Device-independent characterization

The characterization we obtained for the maximal CHSH violation is unique only up to some unavoidable degrees of freedom, encoded in  $\tau_{AB}$  and in the additional subspace  $\mathbb{C}^2 \otimes \mathbb{C}^2$ . Let us first explain where these degrees of freedom come from. Two different quantum realizations can give similar correlators and in particular the following transformations always allow producing new realizations yielding the same statistics:

- Local unitary operations:

$$(\rho, A_x, B_y) \longrightarrow ((U_A \otimes U_B)\rho(U_A \otimes U_B)^\dagger, U_A A_x U_A^\dagger, U_B B_y U_B^\dagger),$$

- Unmeasured additional subspaces:  $(\rho, A_x, B_y) \longrightarrow (\rho \otimes \tau, A_x \otimes \mathbb{1}, B_y \otimes \mathbb{1})$ .

The corresponding correlator vector for all these physically different realization is unchanged. Without any assumption on the local Hilbert space dimension nor on the physical devices being used, it is thus impossible to distinguish between such realizations from the sole knowledge of the correlators. Such a low assumption framework, often called *device-independent* [21], will therefore only be able to give characterizations up to these degrees of freedom.

The fact that some quantum correlations are only achievable by particular states or particular sets of measurements was first observed in seminal works on nonlocality [22, 23]. It was later formalized as *self-testing* [24], under the following definition: when a given correlator vector  $\vec{P}$  can only be achieved, up to local unitary operations and unmeasured additional subspaces, by a unique state and/or measurement, we say that  $\vec{P}$  provides a self-test for this state and/or measurement<sup>1</sup>. If the correlators certify both the state and measurements, we say that it self-tests the corresponding realization. Self-testing in this case is a tool of choice for the study of the quantum set as it implies that  $\vec{P}$  is extremal [26]. Like for the CHSH expression, one way to find such self-test is to find an exposing functional of the quantum set and to prove that the corresponding Tsirelson bound can only be achieved by a ‘unique’ realization. Nevertheless, it is not the only way, as some self-testing statement rely on the full knowledge of the correlators.

Thereby, self-testing appears as promising device-independent tool to characterize physical quantum systems upon minimal assumptions. These are:

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<sup>1</sup>This definition doesn’t take into account the complex conjugation operation, which was proposed later to extend self-testing in scenarios with three or more parties [25].

the physical model is described by quantum mechanics; the non-signaling condition is verified, that is Alice and Bob cannot communicate their inputs to each other; the probabilities are positive and normalized. This makes self-testing rather challenging to perform in practice because of two things:

1. It is impossible to discard any round of the experiment. In practice, it means that Alice and Bob should be able to perform measurements in each run (and not lose a photon, for example). Often referred to as the detection loophole, this condition is required because classical models with post-processing can fake quantum statistics [27].
2. It is required that Alice and Bob cannot have knowledge of the other party's input. Often referred to as the locality loophole, this can be imposed by assumption of physical isolation or by space-like separation of the devices (Alice and Bob should perform their measurements in a short time frame while being at a large distance).

Moreover, every experiment is prone to errors and imperfections. As such, reaching the maximal CHSH value of  $2\sqrt{2}$  is unfeasible in practice. While some characterization of the physical state is still possible for lower violations, most noise-tolerant self-testing protocols known today however impose a CHSH value strictly above 2.106 [28]. Finally, a large number of Bell test trials is needed to avoid the conclusion to be affected by finite size effects of the statistical sample.

Due to all these experimental constraints and even though the theory presented in this first chapter has been developed for many years, experimental results along these lines are still very recent. In the following chapter, we present a work that was done in collaboration with an experimental team in Zurich, which provides the self-testing of a complete quantum realization for the first time.



## II – From the theory to the experiment: Self-testing in practice

The detection loophole was first closed in a self-testing experiment using two ions [29] trapped in a single trap. Four-party GHZ states on a single superconducting circuit device later also closed this loophole [30]. In all these cases, the absence of communication between the nodes relied on physical isolation. Self-testing with space-like separation and closing the detection loophole was first obtained in the posteriori analysis presented in Ref. [31] of the loophole-free Bell test in Ref. [32] using neutral atoms, however only when taking into account data captured over the course of several months.

Furthermore, only the self-testing of quantum states has been demonstrated experimentally so far. However, measurements play an important role in numerous quantum tasks [33]. In fact, their certification through self-testing, alongside the one of the state, is crucial in the certification of the blindness and verifiability property of delegated quantum computing with entangled provers [17, 34–36].

In this chapter, we present a work conducting a *complete self-test* of both a Bell state and pairs of Pauli measurements, in a system of two superconducting circuit devices remotely connected through a 30-meter-long microwave quantum link. Our demonstration closes the detection loophole and ensures the absence of communication between the nodes through space-like separation.

This demonstrates the feasibility of utilizing this fundamentally different verification scheme in a context relevant for building local area networks of remote superconducting circuit quantum processors, with prospects in security and distributed computing. Moreover, enabled by a unique combination of comparably high Bell inequality violations and high data acquisition rates, this implementation achieves the targeted goal in a total experiment time of only about half an hour.

### II.1 - Description of the experimental setup

The experimental setup was performed in Zurich and consists of a two-node system made of two transmon-style superconducting qubits operated in their individual dilution refrigerators at temperatures of about 15 mK. The read out of the state of the qubits is performed using microwave pulses on the nanosecond timescale. The two qubits are connected through a 30-meter-long cryogenically cooled microwave quantum channel, a rectangular waveguide.



uide, used for the distribution of entanglement. The space-like separation of the two qubits at a linear distance of about 30 meters provides a window of about 100 ns for each trial of the experiment, from the generation of the input bits  $x$  and  $y$  to obtaining the measurement outcomes  $a$  and  $b$ , during which the exchange of information between the two nodes is precluded by the laws of special relativity (Fig. II.1). This closes the locality loophole, and in the case of this experiment ensures that no communication occurs between the nodes during the test procedure. Detailed description of the experimental setup can be found in previous works of the Zurich team, see [37, 38].

In each trial of the experiment (Fig. II.1), the entanglement between the two remote qubits is established by having them exchange a single microwave photon through the quantum channel [39]. Once the two qubits are entangled, a random choice of measurement bases for each party is determined by bits provided by trusted random number generators located close to each node of the untrusted setup [40], to support the assumption of measurement independence [41]. At each site, the local random bit controls the untrusted rotation of the qubit in the dilution refrigerator through the conditional application of a microwave pulse, which implements the basis choice selection. Finally, an untrusted single-shot measurement is performed on the two individual qubits [42] and the result is recorded in a trusted memory. The result of all trials are used, which closes the detection loophole.

## II.2 - Robust characterization of states and measurements

In the scenario of interest for this work, the aim is to characterize a state and measurements solely from the CHSH score  $S = \vec{\beta}_{\text{CHSH}} \cdot \vec{P}$ , where  $\vec{P}$  is the distribution observed in the experiment. Although in the case  $S = 2\sqrt{2}$  we do expect that well-defined qubit measurements are performed on a maximally entangled two qubit state, we do not presume that the Hilbert space dimensions and the measurement calibration are known and remain unchanged throughout the experiment. Self-testing defines such a device-independent characterization.

### II.2.1 . Self-testing statement in the ideal case

Let us delve more deeply into self-testing statement within the ideal case where  $S = 2\sqrt{2}$ . Considering the characterization of a bipartite state of an unknown dimension  $\rho_{AB} \in L(\mathcal{H}_A \otimes \mathcal{H}_B)$ , self-testing guarantees the existence of local extraction (completely positive and trace preserving) maps

$$\Lambda_A : L(\mathcal{H}_A) \rightarrow L(\mathbb{C}^2) \quad (\text{II.1})$$

$$\Lambda_B : L(\mathcal{H}_B) \rightarrow L(\mathbb{C}^2) \quad (\text{II.2})$$

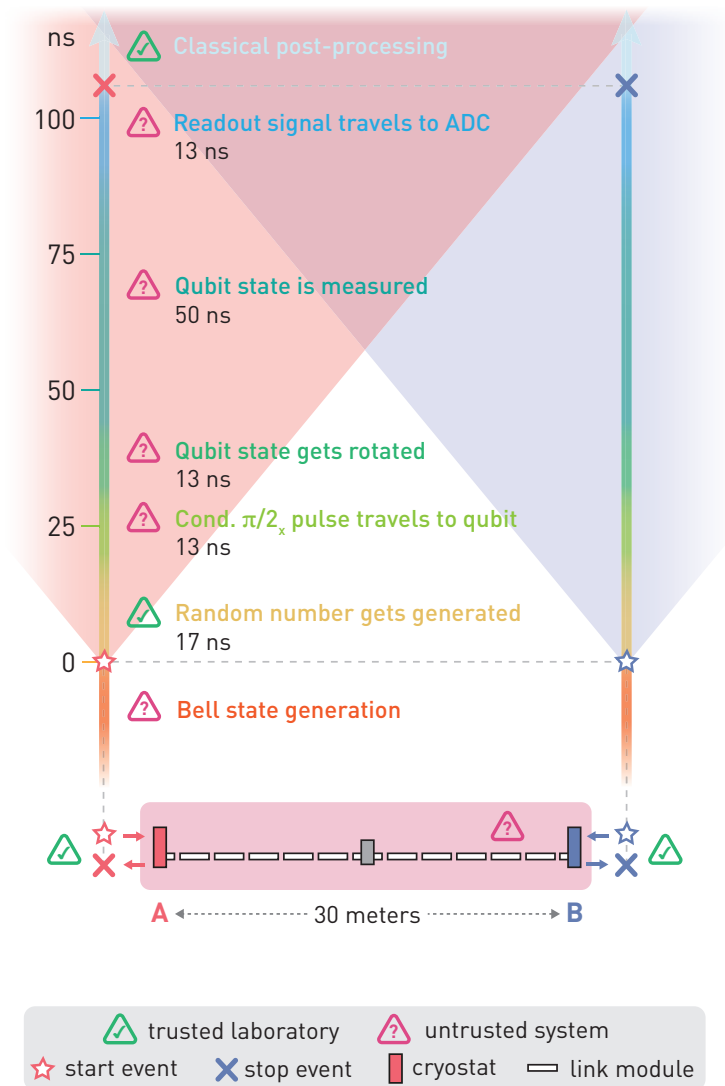


Figure II.1: Self-testing protocol. The figure displays the space-time configuration of a single trial of the experiment. The region shaded in magenta corresponds to the untrusted system under test. The individual steps simultaneously take place on both nodes. The triangular sign marks whether a step takes place as part of the trusted laboratory or of the untrusted system. Stars and crosses mark the start and stop events of each trial, and the shaded red and blue regions the forward light cones of the corresponding start events.

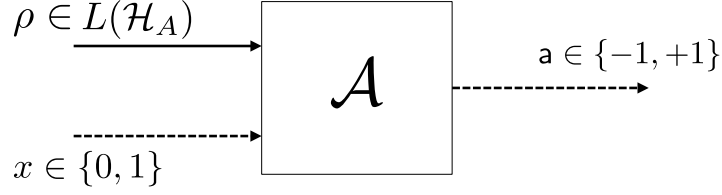


Figure II.2: Schematic description of a measurement apparatus  $\mathcal{A}$  of one party in a Bell-experiment with two inputs and two outputs. Formally speaking, it is a quantum channel with two separated inputs: a classical bit  $x$ , encoding the measurement choice, and a quantum state  $\rho$ , being measured, in an Hilbert space  $\mathcal{H}_A$  of unknown dimension; and one output, consisting of a classical bit  $a$  encoding the measurement outcome.

which identify a sub-system of local dimension 2 in a maximally entangled two qubit state  $|\phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ , that is

$$(\Lambda_A \otimes \Lambda_B)[\rho_{AB}] = |\phi^+\rangle\langle\phi^+|. \quad (\text{II.3})$$

Concerning the characterization of the measurement, Alice's apparatus  $\mathcal{A}$  is described as a device taking as input a state  $\rho_A \in L(\mathcal{H}_A)$  and the measurement setting (a classical value  $x = \{0, 1\}$  in a register labeled by *in*) and giving as output the result of the measurement (a classical value  $a = \{-1, +1\}$  in a register labeled by *out*), see Fig. II.2. In the ideal setting, self-testing guarantees the existence of an injection map

$$V_A : L(\mathbb{C}^2) \rightarrow L(\mathcal{H}_A) \quad (\text{II.4})$$

such that  $\forall \sigma \in L(\mathbb{C}^2)$  and  $\forall x \in \{0, 1\}$ ,

$$(\mathcal{A} \circ V_A)[\sigma \otimes |x\rangle\langle x|_{in}] = \tilde{\mathcal{A}}[\sigma \otimes |x\rangle\langle x|_{in}]. \quad (\text{II.5})$$

The reference apparatus  $\tilde{\mathcal{A}}$  corresponds to a pair of orthogonal Pauli  $\sigma_z$  and  $\sigma_x$  measurements for the setting choice  $x = 0$  and  $x = 1$  respectively, that is

$$\begin{aligned} \tilde{\mathcal{A}}[\sigma \otimes |x\rangle\langle x|_{in}] = & \langle 0 | \sigma | 0 \rangle \langle x | 0 \rangle_{in} | +1 \rangle \langle +1 |_{out} + \langle 1 | \sigma | 1 \rangle \langle x | 0 \rangle_{in} | -1 \rangle \langle -1 |_{out} \\ & + \langle + | \sigma | + \rangle \langle x | 1 \rangle_{in} | +1 \rangle \langle +1 |_{out} + \langle - | \sigma | - \rangle \langle x | 1 \rangle_{in} | -1 \rangle \langle -1 |_{out}. \end{aligned} \quad (\text{II.6})$$

where  $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$ . This characterization of the whole device on Alice, including the input choice, does not only allow one to certify that the action of operators  $A_0$  and  $A_1$  takes place in a given subspace, but also that both measurement basis for input  $x = 0, 1$  are complementary.

In a scenario where Alice shares an entangled state and copies of the input register with a third party, appropriate projections performed by the third

party cover all possible inputs for Alice. The equality in Eq. (II.5) can thus be expressed with a single bipartite quantum state and two input registers of the form  $\rho^+ = |\phi^+\rangle\langle\phi^+| \otimes (|00\rangle\langle 00| + |11\rangle\langle 11|)/2$ , and self-testing guarantees the existence of the map  $V_A$  such that

$$(\mathcal{A} \circ V_A)[\rho^+] = (\tilde{\mathcal{A}})[\rho^+] \quad (\text{II.7})$$

where  $\mathcal{A} \circ V_A$  and  $\tilde{\mathcal{A}}$  operate on Alice's inputs only.

### II.2.2 . State self-testing in the noisy case

The case  $S = 2\sqrt{2}$  that we considered beforehand cannot be realized in an actual experiment due to unavoidable imperfections. Following Ref. [28], we characterize the actual state  $\rho_{AB}$  in a realistic test with  $S < 2\sqrt{2}$  by the best fidelity one can extract with respect to the ideal state  $|\phi^+\rangle$

$$\mathcal{F}(\rho_{AB}, |\phi^+\rangle\langle\phi^+|) = \max_{\Lambda_A, \Lambda_B} F((\Lambda_A \otimes \Lambda_B)\rho_{AB}, |\phi^+\rangle\langle\phi^+|). \quad (\text{II.8})$$

$F$  is the square of the Uhlmann fidelity: for two density matrices  $\tau$  and  $\tau'$ ,  $F(\tau, \tau') = \text{Tr}(\sqrt{\tau^{1/2}\tau'\tau^{1/2}})^2$  which here reduces to the overlap  $F(\tau, \tau') = \text{Tr}[\tau\tau']$  since one of the two states is pure.

To bound  $\mathcal{F}(\rho_{AB}, |\phi^+\rangle\langle\phi^+|)$ , we take into account the fact that the state was used in an experiment leading to a given CHSH score. Interestingly, its infimum over all states compatible with a CHSH score  $S$ , labelled  $\mathcal{F}_s(S)$ , can be lower bounded by

$$\mathcal{F}_s(S) \geq \frac{1}{2} + \frac{1}{2} \cdot \frac{S - S^*}{2\sqrt{2} - S^*} \quad (\text{II.9})$$

where  $S^* = \frac{16+14\sqrt{2}}{17} \approx 2.106$  [28]. This tells us that for any state used to obtain a CHSH score of at least  $S$ , we can extract a bipartite state with local maps whose fidelity to the singlet state is higher than the right-hand side of Ineq. (II.9). This lower bound is plotted in Fig. (II.3).

It is not currently known whether this bound is tight. However, it has been shown that a non-trivial self-testing statement cannot be obtained for any  $S^*$  below  $\approx 2.05$  [43]. Other self-testing bounds could also yield a higher extractability than given by Eq. (II.9) by leveraging more information than the mere CHSH score [44, 45].

### II.2.3 . Measurement self-testing in the noisy case

In the spirit of what has been done for state self-testing, we characterize the actual measurement apparatus in the noisy case  $S < 2\sqrt{2}$  by the best fidelity one can get between  $(\mathcal{A} \circ V_A)[\rho^+]$  and  $\tilde{\mathcal{A}}[\rho^+]$  when maximizing over all injection maps  $V_A$ , that is

$$\mathcal{F}(\mathcal{A}, \tilde{\mathcal{A}}) = \max_{V_A} F((\mathcal{A} \circ V_A)[\rho^+], \tilde{\rho}), \quad (\text{II.10})$$

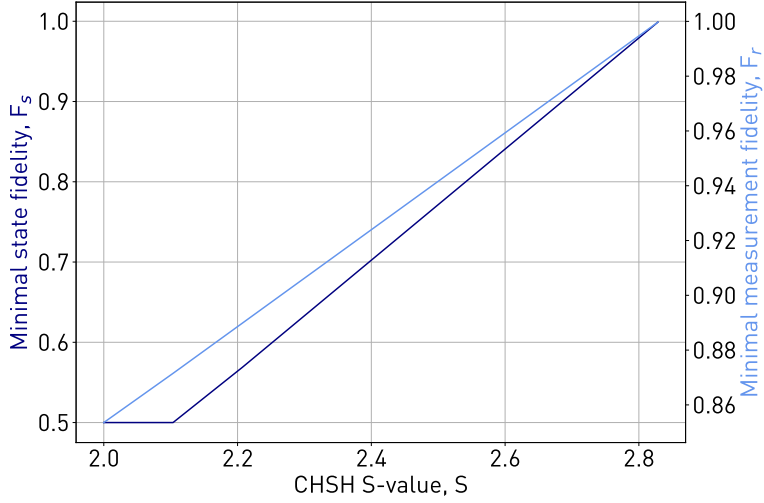


Figure II.3: Minimal Bell state fidelity (dark blue) and measurement fidelity (light blue) certifiable with a given measured CHSH S-value.

where  $\tilde{\rho} := \tilde{\mathcal{A}}[\rho^+]$ . The infimum of  $\mathcal{F}(\mathcal{A}, \tilde{\mathcal{A}})$  over all instruments compatible with a CHSH score  $S$  is labelled  $\mathcal{F}_m(S)$ . Interestingly, we prove that this value can be computed exactly and is given by:

$$\mathcal{F}_m(S) = \frac{\sqrt{2}S + 4}{8}. \quad (\text{II.11})$$

This tells us that for any measurement apparatus  $\mathcal{A}$ , of arbitrary dimension, used to obtain a CHSH score at least  $S$ , there exists a local injection map such that it can be used as the ideal pair of Pauli measurements  $\tilde{\mathcal{A}}$  with a fidelity at least equal to  $\mathcal{F}_m(S)$ . This lower bound is plotted in Fig. (II.3).

The trivial bound for the fidelity is given for  $S = 2$ , that is  $\mathcal{F}_m(2) = \frac{2\sqrt{2}+4}{8} \approx 0.854$ . This value equally corresponds to: the fidelity one can obtain with any apparatus acting on a qubit space by choosing the proper injection; the fidelity attainable by apparatuses that can only give rise to local correlators ( $S \leq 2$ ); the best fidelity one can obtain with an apparatus realizing measurements in only one basis (discarding the classical input bit).

The proof of the bound Eq. (II.11), which can be found in [46, Appendix E], relies on three main results.

1. It suffices to consider measurement apparatuses with a quantum input Hilbert space of dimension 2. Indeed, in a Bell scenario with two binary measurements on each party, one can find local bases in which Alice's and Bob's measurements are block diagonal with blocks of size 2 according to Jordan's lemma. The total CHSH score is the convex mix-

ture of the CHSH score on each qubit-qubit block, and thus there exist at least one block giving a CHSH value higher than the overall one. The freedom on the injection map allows one to inject all the input  $\sigma \in L(\mathbb{C}^2)$  into this specific block.

2. A measurement apparatus with input Hilbert space of dimension 2 can be described with a single parameter  $a$ : up to a local choice of basis, Alice's apparatus performs a  $\sigma_z$ -measurement for input  $x = 0$  and a  $(\cos(a)\sigma_z + \sin(a)\sigma_x)$ -measurement for input  $x = 1$ . The fidelity of such apparatus with respect to the ideal one is given by

$$\mathcal{F}(a) = \frac{1}{4} \left( 2 + \sqrt{2} \cos\left(\frac{a}{2}\right) + \sqrt{2} \sin\left(\frac{a}{2}\right) \right). \quad (\text{II.12})$$

3. A Bell experiment involving the measurement apparatus  $\mathcal{A}(a)$  on Alice's side can only be used to reach CHSH scores up to  $2\sqrt{2} \sin\left(\frac{a}{2} + \frac{\pi}{4}\right)$ . Conversely, when reaching a CHSH score  $S$  and Alice performs qubits measurements, the value of the measurement parameter  $a$  of Alice's apparatus belongs to

$$a \in \left[ 2 \arcsin\left(\frac{S}{2\sqrt{2}}\right) - \frac{\pi}{2}, \frac{3\pi}{2} - 2 \arcsin\left(\frac{S}{2\sqrt{2}}\right) \right]. \quad (\text{II.13})$$

The first point allows one to reduce to the case where  $\mathcal{A}$  input state is a qubit. In this case, it can be described by a single parameter  $a$ , which can be restricted according to the  $S$ -value using the third point. Since the maximal fidelity of any  $\mathcal{A}(a)$  is given by  $\mathcal{F}(a)$ , and this function is symmetric under  $a \rightarrow \pi - a$  and increasing on  $[0, \pi/2]$ , the minimal measurement fidelity value for a CHSH score  $S$  is attained at the lowest possible  $a$  in  $[0, \pi/2]$ . This can be computed explicitly and leads to the bound Eq. (II.11).

The certification schemes we just discussed for the shared Bell state and for the measurement devices provide a mapping between the CHSH  $S$ -value and the certified fidelities. While these formulas are valid for all values of  $S$ , in practice the  $S$ -value that characterizes a setup is never known exactly, and it may even evolve during the course of an experiment. Therefore, a statistical analysis is needed to assess the  $S$ -value that can be supported by a finite number of experimental samples.

### II.3 - Effect of finite size statistics

In order to account for potential parameter fluctuations along the course of an experiment, we assign a different state fidelity  $\mathcal{F}_S^{(i)} := \mathcal{F}(\rho_{AB}^{(i)}, |\phi^+\rangle\langle\phi^+|)$  and measurement fidelity  $\mathcal{F}_M^{(i)} := \mathcal{F}(\mathcal{A}^{(i)}, \tilde{\mathcal{A}})$  to each experimental trial  $i = 1, \dots, n$ , where  $\rho_{AB}^{(i)}$  is the measured state and  $\mathcal{A}^{(i)}$  is the measurement apparatus used by Alice at round  $i$ . These fidelities characterize the quality of

the different parts of the setup at each round. In particular, since the experiment is sequential, i.e. round  $i$  occurs after round  $i-1$ , these fidelities account from memory effects, whereby the behavior of the experiment at round  $i$  may depend on what happened during the previous measurement rounds.

We are interested in bounding the average state and measurement fidelities over the  $n$  measurement trials

$$\mathcal{F}_S^{\text{avg}} = \frac{1}{n} \sum_{i=1}^n \mathcal{F}_S^{(i)}, \quad \mathcal{F}_M^{\text{avg}} = \frac{1}{n} \sum_{i=1}^n \mathcal{F}_M^{(i)}. \quad (\text{II.14})$$

These fidelities can be understood as the average quality of the setup in terms of state and measurement during the course of the actual experiment.

As discussed in earlier sections, both the state and measurement fidelities can be bounded from the CHSH value  $S$ . Writing  $S^{(i)}$  the CHSH score of the system sampled at round  $i$ , the average state fidelity can be bounded as

$$\begin{aligned} \mathcal{F}_S^{\text{avg}} &= \frac{1}{n} \sum_{i=1}^n \mathcal{F}_S^{(i)} \\ &\geq \frac{1}{n} \sum_{i=1}^n \mathcal{F}_s(S^{(i)}) \\ &\stackrel{(\text{II.9})}{\geq} \frac{1}{n} \sum_{i=1}^n \frac{1}{2} + \frac{1}{2} \cdot \frac{S^{(i)} - S^*}{2\sqrt{2} - S^*} \\ &= \frac{1}{2} + \frac{1}{2} \cdot \frac{S^{\text{avg}} - S^*}{2\sqrt{2} - S^*}, \end{aligned} \quad (\text{II.15})$$

i.e. directly from the average CHSH value

$$S^{\text{avg}} = \frac{1}{n} \sum_{i=1}^n S^{(i)}. \quad (\text{II.16})$$

Likewise, the average measurement fidelity can be bounded as

$$\mathcal{F}_M^{\text{avg}} \geq \frac{\sqrt{2}S^{\text{avg}} + 4}{8}, \quad (\text{II.17})$$

using Eq. (II.11). We are thus left with estimating the average CHSH value  $S^{\text{avg}}$  in order to bound  $\mathcal{F}_S^{\text{avg}}$  and  $\mathcal{F}_M^{\text{avg}}$ .

In order to account for finite size effects in the estimation of the average  $S$ -value  $S^{\text{avg}}$ , we compute a lower bound  $S_{\alpha,n}^{\text{avg}} \leq S^{\text{avg}}$  for all possible realizations  $\{S^{(i)}\}_i$  of  $n$  trials with probability at least  $1 - \alpha$ , i.e. with the guarantee that

$$P(S_{\alpha,n}^{\text{avg}} \leq S^{\text{avg}}) \geq 1 - \alpha. \quad (\text{II.18})$$

This defines a trustful one-sided confidence bound on  $S^{\text{avg}}$ . Since Eq. (II.15) and Eq. (II.17) are monotonous in  $S^{\text{avg}}$ , this confidence bound implies lower

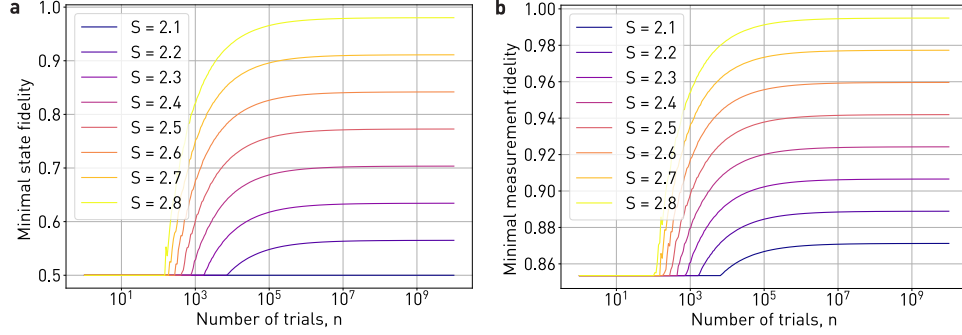


Figure II.4: Dependence of the minimal certifiable state (a) and measurement (b) fidelities given an observed CHSH score  $S$  and the number of experimental trials  $n$  in a self-testing experiment.

confidence bounds on the average fidelities  $\mathcal{F}_S^{\text{avg}}$  and  $\mathcal{F}_M^{\text{avg}}$ , each with confidence  $1 - \alpha$ . We calculate the finite-size-corrected S-value (for  $n$  trials) by employing the method of Ref. [47], which provides a tight lower bound on the average success probability of  $n$  Bernoulli trials. Importantly, this method does not assume that the  $n$  trials are independent and identically distributed (IID). In this context, we introduce the Bell test in the framework of a game. As described further in Ref. [37], in such a setting the two parties A and B aim to win as a team. The game consists of  $n$  rounds. In each trial, A and B individually receive a question, corresponding to a random and uniform input bit  $x$  and  $y$ , and they are asked to reply with a response, corresponding to the measurement outcomes  $a$  and  $b$ . A and B are said to win a certain round of the game if  $x \wedge y = a \oplus b$ , where  $\wedge$  denotes the logical AND function and  $\oplus$  the XOR operation. The winning probability for round  $i$  is given by  $p_i = (4 + S_i)/8$ . The best possible classical strategy allows A and B to achieve a success probability of  $p_{\text{win}}^{\text{LHVM}} = 3/4 = 0.75$ , but a strategy involving shared entanglement achieves higher values, up to  $p_{\text{win}}^{\text{QM}} = \cos^2(\pi/8) \approx 0.854$ .

After all  $n$  trials, we calculate the number of times  $c$  where A and B won the game. For  $\alpha \leq 1/4$ , the lower bound on the average winning probability given  $n$  trials and confidence  $1 - \alpha$  is calculated as [47]

$$p_{\alpha,n}^{\text{avg}} = \begin{cases} c\alpha/n & c \leq 1 \\ I_{\alpha}^{-1}(c, n - c + 1) & c \geq 2 \end{cases}, \quad (\text{II.19})$$

with the inverse of the regularized incomplete Beta function  $I^{-1}$ . The corresponding CHSH S-value is given by

$$S_{\alpha,n}^{\text{avg}} = 8p_{\alpha,n}^{\text{avg}} - 4. \quad (\text{II.20})$$

As a result, small sample sizes yield a substantial reduction of the finite-size-corrected S-value compared to the measured value, and thereby lead to the



certified fidelities being lower. Figure II.4a) displays this behavior for a set of measured  $S$ -values for the certification of a minimal Bell state fidelity, and Fig. II.4b) shows the minimal average measurement fidelity. We observe that finite-size effects substantially matter for small sample sizes  $n \ll 10^7$ , whereas for  $n \geq 10^7$  they become negligible.

## II.4 - Experimental Results

In the main experiment,  $n = 2^{24} \approx 1.67 * 10^7$  trials at a repetition rate of 50 kHz were run. After each  $2^{20} = 1'048'576$  trials, the single-shot readout weights were recalibrated. In total, including software overhead, the experiment took about 40 minutes. Figure II.5 shows the observed CHSH  $S$ -value over the full duration of the protocol. Overall, we recall an average  $S$ -value over the experiment of 2.236, leading to a finite-size corrected  $S$ -value of

$$S_{\text{exp}} = 2.234 \quad (\text{II.21})$$

at a 99% confidence level.

In a fully device-independent context, we can guarantee an average state fidelity of at least  $\mathcal{F}_S^{\text{avg}} \geq 58.9\%$  and an average measurement fidelity of  $\mathcal{F}_M^{\text{avg}} \geq 89.5\%$ , also at a 99% confidence level. The device-independent nature of the experiment is maintained by considering all trials, which closes the fair-sampling loophole, and without assuming the trials to be independent and identically distributed, addressing the memory loophole [27]. Furthermore, we close the communication loophole by space-like separation.

The presented experiment constitutes the first implementation of a complete self-testing that bounds the quality of a distributed entangled state and of the measurement apparatuses at the same time. It also forms the first such implementation with superconducting circuit systems including a clear separation between the nodes, a technology of high relevance for building large-scale quantum computing systems.

While being a relevant quantum information processing task on its own, self-testing is at the heart of other protocols relevant for certifying the security of quantum networks. Potential applications constitute device-independent quantum key distribution [16, 48, 49] and conference key agreement [50], or delegated quantum computing [51]. However, many of these applications involve states and/or measurements that might be different from the ones certified using the CHSH expression. This emphasizes the need for the derivation of self-testing correlators for specific target quantum devices. In the following chapter, we present a method for the derivation of candidate Bell expressions for this task.

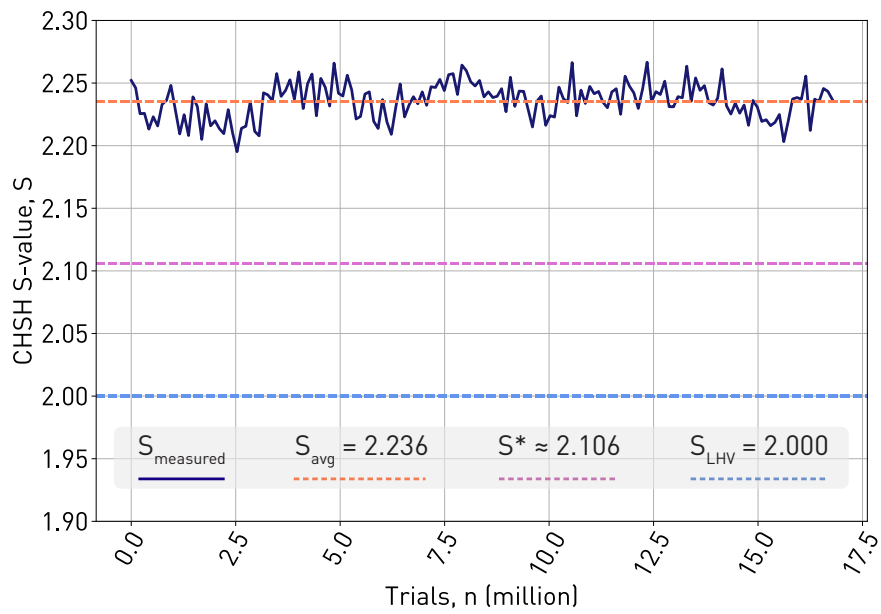


Figure II.5: Recorded CHSH S-value during the full experiment, i.e. all  $n = 2^{24} \approx 16.7$  million trials. The blue curve  $S_{\text{measured}}$  shows the experimental, average S-values of  $2^{17} = 131'072$  trials each. The dashed lines represent the average measured S-value  $S_{\text{avg}}$  of the full dataset, the critical self-testing threshold for the state  $S = S^*$ , and for the measurement (the local bound)  $S_{\text{LHV}}$ .



### III – Custom Bell expressions from formal Sum of Squares

A number of works provided partial answers to the problem of finding relevant Bell expressions for the study of specific states by successfully constructing ones that are maximized by particular target states. Examples include Bell expressions maximized by the maximally entangled state of two qutrits [52–55], and by partially entangled two qubit states [56]. Unfortunately, these approaches rely heavily on the specific structure or symmetry of the target state and do not generalize easily to arbitrary situations.

Other works managed to obtain Bell expressions suited to generic situations by focusing on specific applications of nonlocality. However, these approaches depend on the full probability distributions and rely on the Navascués-Pironio-Acín (NPA) hierarchy [13, 57] to relate to quantum theory. They have thus mostly been considered numerically for given choices of measurements, requiring an a priori guess of the measurements that should be performed on the state of interest to obtain correlations on the boundary of the quantum set.

The study of the self-testing property has also brought a great deal of new Bell expressions along with their Tsirelson bounds [14]. Note that some self-testing results are based on the knowledge of the full measurement statistics rather than solely on the maximal violation of a Bell inequality [24, 58–61]. Whereas self-tests based on full statistics rely on numerous parameters, the ones based on a single quantity may be easier to use and lead to a wide range of applications, as in the case of partially entangled states self-tested from the tilted CHSH expression [59, 60, 62–64]. Constructing simple Tsirelson inequalities is thus relevant even for states already known to be self-testable.

Among the techniques developed for self-testing, sum of squares (SOS) play an important role [14, 65, 66]. Indeed, significant properties of a Bell expression such as its Tsirelson bound can be inferred from its sum of squares decomposition [67]. Sum of squares have also been used to construct Tsirelson inequalities from a fixed choice of quantum state and measurements [55, 68–70]. Finally, the self-testing property itself was used to construct Bell expressions, potentially for arbitrary multipartite states [64]. While generic, this last method also relies on the usage of a choice of the measurements. Therefore, no method for constructing Bell expressions tailored to a specific quantum state is known that is really generic, analytical and flexible.

Here, we present a systematic method that enables the construction of Bell expressions for generic target quantum states with the guarantee that

the state reaches its maximal quantum value. To do so, we introduce a formalism based on polynomial algebra that allows to build directly Bell expressions from SOS decompositions. We apply this method to several cases and discuss the relation of the obtained Tsirelson inequalities to self-testing.

### III.1 - Formal polynomials

Let  $\{X_i\}_i$  be a set of indeterminates in an associative algebra over a field  $\mathbb{K}$ . A *formal multivariate polynomial* is a linear combination [71]

$$S = \sum_i \alpha_i M_i \quad (\text{III.1})$$

where  $M_i$  are monomials, i.e. products of indeterminates such as  $X_1$ ,  $X_1 X_2$  or  $X_1^2 X_2 X_1$ , weighted by scalars  $\alpha_i \in \mathbb{K}$ .

Considering the algebra  $\mathcal{R}$  induced by the  $(n, m, k)$ -Bell scenario, we associate to the outcome  $a$  of the measurement  $x$  of the party  $j$  the indeterminate  $X_{a|x}^{(j)}$ . These indeterminates, also called 'non-commuting variables', obey the algebraic rules of

$$\text{Hermiticity:} \quad \left(X_{a|x}^{(j)}\right)^\dagger = X_{a|x}^{(j)} \quad (\text{III.2a})$$

$$\text{Orthogonality:} \quad X_{a|x}^{(j)} X_{a'|x}^{(j)} = \delta_{a,a'} X_{a|x}^{(j)} \quad (\text{III.2b})$$

$$\text{Normalization:} \quad \sum_a X_{a|x}^{(j)} = 1 \quad (\text{III.2c})$$

$$\text{Commutation:} \quad [X_{a|x}^{(j)}, X_{a'|x'}^{(j')}] = 0 \text{ for } j \neq j'. \quad (\text{III.2d})$$

In this algebra, any monomial  $M_i$  can always be written as the product of  $n$  multivariate monomials  $M_i^{(j)}$  involving indeterminates from each party individually:

$$M_i[\{X_{a|x}^{(j)}\}] = M_i^{(1)}[\{X_{a|x}^{(1)}\}] \dots M_i^{(n)}[\{X_{a|x}^{(n)}\}]. \quad (\text{III.3})$$

When all monomials  $M_i^{(j)}$  in the polynomial  $S$  are of degree one, we say that  $S$  is of *local degree 1* [72]. To any such polynomial

$$S = \sum_{\vec{a}|\vec{x}} \alpha_{\vec{a}|\vec{x}} X_{a|x}^{(1)} \dots X_{a|x}^{(n)} \quad (\text{III.4})$$

we can associate a Bell expression  $\vec{\beta} = \{\alpha_{\vec{a}|\vec{x}}\}_{\vec{a}|\vec{x}}$ . As such, the value of the Bell expression on a given realization  $(|\psi\rangle, \{\Pi_{a|x}^{(j)}\}_{a,x,j})$  can be computed as

$$\vec{\beta} \cdot \vec{P} = \langle \psi | \hat{S} | \psi \rangle \quad (\text{III.5})$$

where the Bell operator is given by  $\hat{S} = S(\{\Pi_{a|x}^{(j)}\})$ , and corresponds to the evaluation of the formal polynomial  $S$  on the specific choice of measurements.

This identification is reversible, defining for each Bell expression a corresponding unique formal polynomial. We thus refer to polynomials with local degree 1 as *formal Bell polynomials*. As an example, the formal CHSH polynomial associated to the CHSH inequality (defined in Eq. (I.14)) is given by

$$\beta_{\text{CHSH}} = \sum_{\substack{\mathbf{a}_1, \mathbf{a}_2 \in \{-1, 1\} \\ x_1, x_2 \in \{0, 1\}}} \mathbf{a}_1 \mathbf{a}_2 (-1)^{x_1 x_2} X_{\mathbf{a}_1 | x_1}^{(1)} X_{\mathbf{a}_2 | x_2}^{(2)}. \quad (\text{III.6})$$

Just like it is sometimes more convenient to parametrize measurements by the combination of projectors, it is sometimes useful to represent a formal polynomial in terms of different indeterminates than the ones associated with measurement projection operators. For instance, each measurement  $x$  of party  $j$  can be described by the single operator

$$Y_x^{(j)} = \sum_{\mathbf{a}=0}^{k-1} w_k^{\mathbf{a}} X_{\mathbf{a}|x}^{(j)}, \quad (\text{III.7})$$

where  $w_k = \exp(2i\pi/k)$ , obtained by applying the Fourier transform on all indeterminates associated with the different outcomes of the measurement. By construction, the  $d$ -th power of  $Y_x^{(j)}$  is 1, and all the indeterminates  $X_{\mathbf{a}|x}^{(j)}$  can be expressed as a linear combination of the powers of  $Y_x^{(j)}$ . Note that this requires considering a complex field  $\mathbb{K}$  when  $j > 2$ . The new indeterminates  $Y_x^{(j)}$  are unitary in the sense that  $(Y_x^{(j)})^\dagger Y_x^{(j)} = Y_x^{(j)} (Y_x^{(j)})^\dagger = 1$ . In this new basis, the CHSH polynomial can be written

$$\beta_{\text{CHSH}} = A_0 B_0 + A_0 B_1 + A_1 B_0 - A_1 B_1, \quad (\text{III.8})$$

where we used a more elegant notation for the indeterminates  $A_x = Y_x^{(0)}$  and  $B_y = Y_y^{(1)}$  in the bipartite case. Note that the Fourier indeterminates are also Hermitian  $A_x^\dagger = A_x, B_x^\dagger = B_x$  in the case of binary measurements ( $d = 2$ ).

Since they provide a description of Bell expressions independently of a specific quantum implementation, formal polynomials on non-commuting variables provide a powerful tool for their analysis. In particular, formal polynomials can be used to compute Tsirelson bounds of Bell expressions, i.e. bounds on the maximal quantum value achievable that is valid independently of the quantum state, measurement and Hilbert space dimension.

As an example, it is known that the CHSH polynomial can be written as the following sum of squares [14, 34, 65, 67]:

$$2\sqrt{2} - \beta_{\text{CHSH}} = \frac{1}{\sqrt{2}} \left[ \left( A_0 - \frac{B_0 + B_1}{\sqrt{2}} \right)^2 + \left( A_1 - \frac{B_0 - B_1}{\sqrt{2}} \right)^2 \right]. \quad (\text{III.9})$$

Since the square of a polynomial  $S^\dagger S$  can only result in a positive contribution, this directly implies that the maximal value of the corresponding CHSH

expression achievable upon measurement of any quantum state is limited to  $2\sqrt{2}$ . In other words, polynomial inequalities

$$\beta \preceq C \quad (\text{III.10})$$

on formal Bell polynomials  $\beta$ , where  $C$  is a real number, imply a Tsirelson bound on the corresponding Bell expression: for all possible statistics  $\vec{P}$  obtained by quantum mechanics, the associated Bell expression  $\vec{\beta}$  verifies

$$\vec{\beta} \cdot \vec{P} \leq C. \quad (\text{III.11})$$

### III.2 - SOS method

Our goal is now to find a consistent method to derive a Bell expression that is maximized by a realization of interest  $(|\psi\rangle, \{\Pi_{a|x}^{(k)}\}_{a,x,k})$ , fixed for the rest of the enunciation of the method. We denote by  $\vec{P}$  the correlator vector corresponding to this realization. Formally speaking, our goal is to find a vector  $\vec{\beta}$  such that

$$\vec{\beta} \cdot \vec{P} = \beta_{\mathcal{Q}} \quad (\text{III.12})$$

where  $\beta_{\mathcal{Q}}$  is the maximum quantum value of  $\vec{\beta}$ . Up to re-normalization, one can always take it to be 1.

For a given candidate  $\vec{\beta}$ , the first thing to ensure is that its quantum bound is indeed 1. Considering the formal Bell polynomial  $\beta$  associated to  $\vec{\beta}$ , a sufficient condition to have  $\vec{\beta} \cdot \vec{P} \leq 1$  for all  $\vec{P} \in \mathcal{Q}$  is that  $1 - \beta$  is a sum of squares (SOS):

$$1 - \beta = \sum_i N_i^\dagger N_i, \quad (\text{III.13})$$

where  $N_i$  are arbitrary formal polynomials. This is known as an SOS relaxation [73, 74]. However, the search space of all formal polynomials  $\mathcal{R}$  is of infinite dimension. Since an SOS decomposition of the form of Eq. (III.13) where  $N_i$  are restricted to a set subspace  $\mathcal{T} \subset \mathcal{R}$  still provides a valid bound, a common approach to tackle this problem consists in considering operators  $N_i$  within a chosen relaxation level  $\mathcal{T}$ , such as the set of all polynomials of a given degree. But even this quickly results in a large problem.

To further reduce the SOS search space, let us use the fact that the correlations  $\vec{P}$  should reach the maximal value to identify a relevant subspace of  $\mathcal{T}$  in which the operators  $N_i$  should be chosen. If a SOS decomposition of the form Eq. (III.13) exists, this would imply:

$$0 = \sum_i \langle \psi | \hat{N}_i^\dagger \hat{N}_i | \psi \rangle = \sum_i \| \hat{N}_i | \psi \rangle \|^2, \quad (\text{III.14})$$

where  $\hat{N}_i$  is the evaluation of  $N_i$  on our choice of measurements. Since all terms on the right-hand side of the above equation are positive, this implies

that for all  $i$ ,  $\hat{N}_i |\psi\rangle = 0$ , i.e. that all  $\hat{N}_i$  are nullifying operators of  $|\psi\rangle$  [65]. This condition restricts the operators  $N_i$  to

$$\mathcal{A}_{\mathcal{T}} = \{N \in \mathcal{T} : \hat{N} |\psi\rangle = 0\}. \quad (\text{III.15})$$

For a finite relaxation  $\mathcal{T}$ , let's consider a generating sequence  $\{N_s\}_s$  of  $\mathcal{A}_{\mathcal{T}}$  and denote by  $\vec{N}$  the vector of elements  $N_s$ . All elements in  $\mathcal{A}_{\mathcal{T}}$  can thus be written as  $\vec{w} \cdot \vec{N}$  where  $\vec{w}$  is a real vector. A valid SOS decomposition in  $\mathcal{T}$  can then be written as

$$1 - \beta = \sum_s O_s^\dagger O_s = \vec{N}^\dagger \sum_s \vec{w}_s^\dagger \vec{w}_s \vec{N} = \vec{N}^\dagger \cdot W \cdot \vec{N}, \quad (\text{III.16})$$

where  $W = \sum_s \vec{w}_s^\dagger \vec{w}_s$  is a positive matrix. We see that the problem of obtaining an SOS decomposition reduces to finding whether there exists a matrix  $W$  such that

$$1 - \beta = \vec{N}^\dagger \cdot W \cdot \vec{N}, \quad (\text{III.17a})$$

$$W \succeq 0. \quad (\text{III.17b})$$

If such a matrix  $W$  can be found, we say it is a certificate of the expression  $\vec{\beta}$ .

However, in all generality, for an arbitrary matrix  $W \succeq 0$ , the right-hand term of Eq. (III.17b) is not equal to a formal polynomial of local degree higher than 1 and the condition  $W \succeq 0$  can be hard to parameterize. In order to find a single solution to the problem, one may consider a finite number of (possibly parameterized) polynomials  $N_i \in \mathcal{A}_{\mathcal{T}}$ . In general for arbitrary polynomials  $N_i$ , the resulting sum of squares will give

$$\sum_i N_i^\dagger N_i = C - \beta + \Gamma, \quad (\text{III.18})$$

where  $C$  is a real number,  $\beta$  is a formal Bell polynomial (to which we can associate a Bell expression), and  $\Gamma$  is some leftover polynomial term of higher local order. This last term needs to vanish in order to have a valid sum of squares decomposition. The "condition" of the sum of squares method thus take the simple form

$$\Gamma = 0. \quad (\text{III.19})$$

and comes down to solving a quadratic system. This leads us to formulate the following SOS method for the construction of Bell expressions suited for a specific target state.

1. Choose a set of operators  $\hat{N}_i$  that are nullifying the target state, i.e. such that  $|\psi\rangle \in \cap_i \ker(\hat{N}_i)$ , and in particular

$$\hat{N}_i |\psi\rangle = 0 \quad \forall i. \quad (\text{III.20})$$



2. Parameterize measurement bases  $\hat{M}_x^{(i)}$  for each party.
3. Choose a relaxation  $\mathcal{T}$  and find the elements  $N_i$  inside this relaxation whose evaluation on the measurements  $\hat{M}_x^{(i)}$  correspond to the nullifiers  $\hat{N}_i$ .
4. Compute the sum of squares Eq. (III.18) on the polynomials  $N_i$ .
5. Solve the condition that all terms of local order higher than one vanishes

$$\Gamma = 0. \quad (\text{III.21})$$

Note that the promotion of the nullifiers from the operator space to the formal polynomial algebra performed in Step 3 before computing the sum of squares is a key ingredient of the SOS method. While the choice space of the nullifiers  $\hat{N}_i$  only depends on the target state, this mapping from the operators  $\hat{N}_i$  to formal polynomials  $N_i$  depends on the choice of measurements and is not unique. Therefore, one has to choose how to do this lifting operation: the number of possible different lifts depends on the relaxation  $\mathcal{T}$  for the polynomials  $N_i$ . As such, one could choose only one polynomial  $N_i \in \mathcal{T}$  for each  $\hat{N}_i$  (if there exists one) or all such  $N_i$  to compute the SOS. Note that if the chosen relaxation of polynomials is of local degree 1 (the almost quantum level [57]) and the measurements are linearly independent for each party (for instance when dealing with two qubit measurements per party), the correspondence between  $\hat{N}_i$  and  $N_i$  is one-to-one: one can simply express the nullifiers in terms of the measurement operators  $\hat{M}_x^{(i)}$  and define the corresponding formal polynomial by promoting the measurement operators to indeterminates  $\hat{M}_x^{(i)} \rightarrow M_x^{(i)}$ .

We also want to highlight the fact that the sum of square method can be used to construct expressions tailored to target measurements as well, such as families of Bell expressions for fixed settings and varying states [75]. For example, the choice of measurement in Step 2 could be fixed beforehand, and Step 1 would consist of finding a family of operators  $\hat{N}_i(\vec{\theta})$  inside the algebra generated by the  $\{\hat{M}_x^{(i)}\}$  nullifying a parametrized state  $|\psi(\vec{\theta})\rangle$ .

The SOS method guarantees that no implementation can provide a larger Bell value than the target one. It is thus a *sufficient condition* to construct a Bell expression for a target quantum state: any expression verifying  $\Gamma = 0$  is maximized by the considered state. The method relies on a choice of operators, here nullifiers, and of measurements. Therefore, a candidate that does not verify the SOS condition Eq. (III.19) for a specific choice of  $\hat{N}_i$  and  $\hat{M}_x^{(i)}$  is not automatically ruled out, as it might admit a valid SOS decomposition for another choice.

It is however known that finding the SOS decomposition of a formal Bell polynomial [67] is dual to the NPA hierarchy [57], which converges in the limit

of the hierarchy. This limit corresponds to considering the full space of formal polynomials with no limit on the number of squares nor on the monomial length. Thus, if one considers all possible choices of formal nullifiers for monomial length  $n$ , and completely parametrizes the finite dimensional measurements, the SOS method becomes *necessary and sufficient* in the asymptotic limit  $n \rightarrow \infty$ . This means that a Bell expression can be maximized by the considered state if and only if there exists a choice of measurements and an asymptotic choice of nullifiers such that  $\Gamma = 0$ . In this sense, the SOS method is *asymptotically complete*.

Finally, we remark that the strength of this method is not only to construct Bell expressions whose Tsirelson bound is reached by the target state. By also providing their sum of squares decomposition, conditions on the action of the measurements on the state are also obtained: the operators  $\hat{N}_i$  nullify the state for any implementation reaching the quantum bound. This is interesting as for an arbitrary Bell expression, it is in general hard to find its Tsirelson bound or its SOS decomposition. Moreover, many proofs of self-testing rely on the sum of squares decomposition of the Bell expression [14].

### III.3 - New Bell expressions for the maximally entangled state of two qutrits

In this section, we apply the SOS method to the case of the maximally entangled state of two qutrits

$$|\psi^3\rangle = \frac{|00\rangle + |11\rangle + |22\rangle}{\sqrt{3}}. \quad (\text{III.22})$$

In general, it may be difficult to apply the method on a full parametrization of the measurement bases for large Hilbert space dimension. But the Bell expressions provided by the method are maximized by the desired state even when the measurement bases considered are not fully parametrized. We thus consider a family of measurements which generalizes the ones first used in [76] to maximize the CGLMP expression, and then in [55, 77] to self-test the maximally entangled two qutrits state. Namely, we consider a Bell scenario where Alice and Bob each have two inputs and three outputs. For  $x, y \in \{0, 1\}$  we choose measurement bases of the form

$$\hat{\Pi}_{\mathbf{a}|x} = U(a_x)F^\dagger |\mathbf{a}\rangle\langle\mathbf{a}| FU(a_x)^\dagger \quad (\text{III.23a})$$

$$\hat{\Pi}_{\mathbf{b}|y} = U(b_y)F^\dagger |\mathbf{b}\rangle\langle\mathbf{b}| FU(b_y)^\dagger \quad (\text{III.23b})$$

These bases are related to the computational one by the Fourier transform

$$F = \frac{1}{\sqrt{3}} \sum_{k,l=0}^2 w^{kl} |k\rangle\langle l| \quad \text{with} \quad w = \exp(2i\pi/3) \quad (\text{III.24})$$

followed by a phase rotation with a real parameter  $\theta$

$$U(\theta) = \sum_{k=0}^2 w^{k\theta} |k\rangle\langle k|. \quad (\text{III.25})$$

By analogy with the case of formal polynomials in Eq. (III.7), we define the unitary operators associated to each measurement by

$$\hat{A}_x = \sum_{a=0}^2 w^a \hat{\Pi}_{a|x} = \begin{pmatrix} 0 & 0 & w^{-2a_x} \\ w^{a_x} & 0 & 0 \\ 0 & w^{a_x} & 0 \end{pmatrix}, \quad (\text{III.26a})$$

$$\hat{B}_y = \sum_{b=0}^2 w^b \hat{\Pi}_{b|y} = \begin{pmatrix} 0 & 0 & w^{-2b_y} \\ w^{b_y} & 0 & 0 \\ 0 & w^{b_y} & 0 \end{pmatrix}. \quad (\text{III.26b})$$

In the case of qutrits these operators verify  $A_x^\dagger = A_x^2$ , and any projector  $\hat{\Pi}_{a|x}$  can be expressed as a linear combination of the identity operator,  $A_x$  and  $A_x^\dagger$ , likewise for Bob.

The first step of the SOS method is to find nullifiers for the target state. To do so, we exploit the fact that for any unitary operator  $\hat{M}$  the following identity holds:

$$\hat{M} \otimes \hat{M}^* |\psi^3\rangle = |\psi^3\rangle, \quad (\text{III.27})$$

where  $\hat{M}^*$  is the complex conjugate of  $\hat{M}$ . Thus, we decide to consider two nullifying operators of the form

$$\hat{N}_x = \mathbb{1} - \hat{A}_x \otimes \hat{B}_x, \quad x \in \{0, 1\}, \quad (\text{III.28})$$

such that the operators  $\hat{B}_x$  verify

$$\hat{B}_x = \hat{A}_x^* \quad (\text{III.29})$$

when acting on Alice's Hilbert space.

The most general way to construct these operators from Bob's measurement operators is to take

$$\hat{B}_x = c_x \mathbb{1} + \mu_{0,x} \hat{B}_0 + \mu_{1,x} \hat{B}_1 + \nu_{0,x} \hat{B}_0^2 + \nu_{1,x} \hat{B}_1^2. \quad (\text{III.30})$$

Now, together with equation (III.29), this implies that  $c_x = \nu_{0,x} = \nu_{1,x} = 0$  and

$$\begin{cases} \mu_{0,x} w^{b_0} + \mu_{1,x} w^{b_1} = w^{-a_x} \\ \mu_{0,x} w^{-2b_0} + \mu_{1,x} w^{-2b_1} = w^{2a_x}. \end{cases} \quad (\text{III.31})$$

With simple algebra this system of equation solves to

$$\begin{cases} \mu_{0,x} = \frac{w^{2a_x} - w^{-a_x-3b_1}}{w^{-2b_0} - w^{b_0-3b_1}} \\ \mu_{1,x} = \frac{w^{2a_x} - w^{-a_x-3b_0}}{w^{-2b_1} - w^{b_1-3b_0}}. \end{cases} \quad (\text{III.32})$$

Now that we defined our two nullifiers we need to lift them to the formal polynomial formalism. We decide to take polynomials  $N_x = \mathbb{1} - A_x \otimes \overline{B_x}$  and compute the sum of squares  $pN_0^\dagger N_0 + (1-p)N_1^\dagger N_1$  for an arbitrary  $p \in (0, 1)$  (the limit cases  $p = 0, 1$  where only one nullifier appears would be insufficient to grant self-testing because several states are in the kernel of the nullifying operator). When developing the squares we get:

$$pN_0^\dagger N_0 + (1-p)N_1^\dagger N_1 = C - \hat{S} + \hat{\Gamma}, \quad (\text{III.33})$$

where  $C = 2$ ,  $\beta$  is a formal polynomial of local degree 1 and  $\Gamma$  is the leftover of higher local degree given here by

$$\Gamma = (p\mu_{0,0}^* \mu_{1,0} + (1-p)\mu_{0,1}^* \mu_{1,1}) B_0^\dagger B_1 + h.c. \quad (\text{III.34})$$

where  $h.c.$  denotes the Hermitian conjugate of the first part. Following the SOS method, we look for the parameter regime where the leftover term  $\Gamma$  vanishes. This is the case when

$$p\mu_{0,0}^* \mu_{1,0} + (1-p)\mu_{0,1}^* \mu_{1,1} = 0. \quad (\text{III.35})$$

This can be written as a condition on the measurements parameters  $a_x, b_y$  and leads to

$$p \sin(\pi(a_0 + b_1)) \sin(\pi(a_0 + b_0)) + (1-p) \sin(\pi(a_1 + b_1)) \sin(\pi(a_1 + b_0)) = 0. \quad (\text{III.36})$$

We thus obtain a family of Bell expressions, with their Tsirelson bound, given by:

$$\beta = pA_0\overline{B_0} + (1-p)A_1\overline{B_1} + h.c. \preceq 2, \quad (\text{III.37})$$

where  $\overline{B_x} = \mu_{0,x}B_0 + \mu_{1,x}B_1$  and coefficient  $\mu_{y,x}$  are given by equations (III.32). Here,  $a_x, b_y$  and  $p$  are free parameters constrained only by Eq. (III.36). Without loss of generality we can set  $a_0 = 0$  and  $-b_0 < -b_1$ , and choose  $a_1, -b_0, -b_1$  in  $[0, \pi)$ . Eq. (III.36) then implies the alternating condition  $-b_0 < a_1 < -b_1$  in analogy with the maximally entangled qubit state [78]. Note that the average value of  $\beta$  over any state is real, as the Hermitian conjugate ( $h.c.$ ) part ensures that  $\beta$  is a Hermitian polynomial.

One expression among the ones we found, for parameters  $a_0 = 0, a_1 = 1/2, b_0 = 1/4, b_1 = 3/4$ , was already known and has been proven to self-tests the maximally entangled state of two qutrits along with the associated measurements [55, 77]. It would be interesting to see whether one can generalize their self-testing argument to the family of Bell expressions we discovered.

## III.4 - Self-tests for the partially entangled two-qubit states

### III.4.1 . A two-parameter family of self-tests based on three nullifiers

In this section, we look at partially entangled two qubit states

$$|\phi_\theta\rangle = c_\theta |00\rangle + s_\theta |11\rangle, \quad (\text{III.38})$$

where we use the notation  $c_\theta = \cos(\theta)$ ,  $s_\theta = \sin(\theta)$ . We consider the following nullifying operators

$$\begin{cases} \hat{N}_0 = \hat{Z}_A - \hat{Z}_B, \\ \hat{N}_1 = \hat{X}_A - s_{2\theta}\hat{X}_B - c_{2\theta}\hat{X}_A\hat{Z}_B. \\ \hat{N}_2 = 1 - s_{2\theta}\hat{X}_A\hat{X}_B - c_{2\theta}\hat{Z}_B \end{cases} \quad (\text{III.39})$$

where  $\hat{Z}_{A(B)}$  and  $\hat{X}_{A(B)}$  denote the Pauli  $z$  and  $x$  on Alice(Bob) Hilbert space respectively. We parameterize the measurement operators for Alice and Bob respectively as

$$\begin{cases} \hat{A}_0 = \hat{Z}_A, & \hat{A}_1 = \hat{X}_A, \\ \hat{B}_y = \cos(b_y)\hat{Z}_B + \sin(b_y)\hat{X}_B. \end{cases} \quad (\text{III.40})$$

where angles  $b_1$  and  $-b_0$  might be different. Note that up to relabelling of measurement incomes and/or outcomes, we can always assume that  $b_1, b_0 \in [-\pi/2, \pi/2]$  and  $b_1 < b_0$ .

We decide to apply the method at the almost quantum level. As such, we express the nullifiers in terms of the measurement operators, and promote them to formal polynomials as follows:

$$N_0 = A_0 - \frac{\sin(b_0)B_1 - \sin(b_1)B_0}{\sin(b_0 - b_1)}, \quad (\text{III.41a})$$

$$N_1 = A_1 - s_{2\theta} \frac{-\cos(b_0)B_1 + \cos(b_1)B_0}{\sin(b_0 - b_1)} - c_{2\theta}A_1 \frac{\sin(b_0)B_1 - \sin(b_1)B_0}{\sin(b_0 - b_1)},$$

$$N_2 = 1 - s_{2\theta}A_1 \frac{-\cos(b_0)B_1 + \cos(b_1)B_0}{\sin(b_0 - b_1)} - c_{2\theta} \frac{\sin(b_0)B_1 - \sin(b_1)B_0}{\sin(b_0 - b_1)}.$$

We consider an SOS of the form  $N_0^2 + (\lambda_1 N_1 + \lambda_2 N_2)^2$  for real parameters  $\lambda_1$  and  $\lambda_2$ . When developing the squares we obtain terms proportional to the anti-commutator  $\{B_1, B_0\}$  and to  $A_1\{B_1, B_0\}$  which contribute to  $\Gamma$ . The conditions  $\Gamma = 0$  then leads to two equations:

$$\alpha(\lambda_1^2 + \lambda_2^2) + 2\beta\lambda_1\lambda_2 = 0, \quad (\text{III.42a})$$

$$\beta(\lambda_1^2 + \lambda_2^2) + 2\alpha\lambda_1\lambda_2 = -s_{b_1}s_{b_0}, \quad (\text{III.42b})$$

with

$$\alpha = -\frac{1}{2}s_{4\theta}s_{b_1+b_0}, \quad \beta = s_{2\theta}^2c_{b_1}c_{b_0} + c_{2\theta}^2s_{b_1}s_{b_0}. \quad (\text{III.43a})$$

These two equations admit a solution when Bob's measurements lie in the squared region:

$$[b_1 \in (-2\theta, 0), b_0 \in (0, 2\theta)]. \quad (\text{III.44a})$$

The sum of square decomposition is then given by:

$$N_0^2 + (\lambda_1 N_1 + \lambda_2 N_2)^2 = C(\theta, b_0, b_1) - \beta_{\theta, b_0, b_1} \quad (\text{III.45})$$

where:

$$\begin{aligned} \beta_{\theta, b_0, b_1} = & 2A_0 \frac{s_{b_0} B_1 - s_{b_1} B_0}{s_{b_0 - b_1}} \\ & - 4\lambda_1 \lambda_2 \left[ A_1 - s_{2\theta} \frac{-c_{b_0} B_1 + c_{b_1} B_0}{s_{b_0 - b_1}} - c_{2\theta} A_1 \frac{s_{b_0} B_1 - s_{b_1} B_0}{s_{b_0 - b_1}} \right] \\ & + 2(\lambda_1^2 + \lambda_2^2) \left[ s_{2\theta} A_1 \frac{-c_{b_0} B_1 + c_{b_1} B_0}{s_{b_0 - b_1}} + c_{2\theta} \frac{s_{b_0} B_1 - s_{b_1} B_0}{s_{b_0 - b_1}} \right], \quad (\text{III.46}) \\ C(\theta, b_0, b_1) = & 2(1 + \lambda_1^2 + \lambda_2^2) \end{aligned}$$

and

$$\lambda_1 \lambda_2 = -\frac{s_{b_1} s_{b_0} s_{b_1 + b_0} s_{4\theta}}{(c_{2b_1} - c_{4\theta})(c_{2b_0} - c_{4\theta})}, \quad (\text{III.47a})$$

$$\lambda_1^2 + \lambda_2^2 = -\frac{4s_{b_1}^2 s_{b_0}^2 (c_{2\theta}^2 + \cot(b_1) \cot(b_0) s_{2\theta}^2)}{(c_{2b_1} - c_{4\theta})(c_{2b_0} - c_{4\theta})}. \quad (\text{III.47b})$$

The new candidate Bell expressions with associated Tsirelson bound are given by

$$\beta_{\theta, b_0, b_1} \preceq C(\theta, b_0, b_1). \quad (\text{III.48})$$

These new expressions can be used to self-test the partially entangled state when Alice performs measurements  $\hat{Z}_A$  and  $\hat{X}_A$ , and Bob performs any measurement in the  $(\hat{Z}_B, \hat{X}_B)$ -plane with  $b_0 \in (0, 2 * \theta)$ ,  $b_1 \in (-2 * \theta, 0)$ . The proof of the self-test relies on the algebraic relations one can derive from the fact that every realization reaching the Tsirelson bound of the new Bell expression satisfies  $\hat{N}_0 |\psi\rangle = (\lambda_1 \hat{N}_1 + \lambda_2 \hat{N}_2) |\psi\rangle = 0$ .

In the case where Alice's measurements are given by  $\hat{Z}_A$  and  $\hat{X}_A$ , the settings given by Eq. (III.44) seem to be the only ones allowing to self-test the partially-entangled state  $|\phi_\theta\rangle$ . Indeed, we verify numerically that any other choice of measurement settings for Bob results in behaviors that do not lie on the boundary of the NPA relaxation set at local level  $\ell = 1$ . For this, we consider the following optimization

$$\begin{aligned} \Delta = & \min_i \max_{\vec{P}_1, \vec{P}_2} \vec{P}_1^i - \vec{P}_2^i \\ \text{s.t. } & \vec{P}_1^j = \vec{P}_2^j = \vec{P}^j, \quad j \neq i \\ & \vec{P}_1, \vec{P}_2 \in \text{NPA}_\ell \end{aligned} \quad (\text{III.49})$$

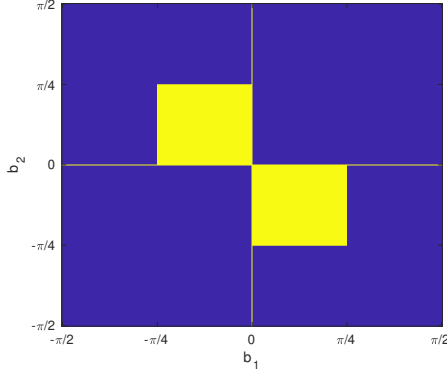


Figure III.1: Result of the optimization Eq. (III.49) for various choice of measurement angles for Bob. Points with  $\Delta \leq 10^{-11}$  in yellow are on the boundary of the quantum set. Except when  $b_1 = 0$  or  $b_0 = 0$ , in which case the behavior admits a probability equal to zero (both Alice and Bob measure in the  $\hat{Z}$  direction), all points outside the interval Eq. (III.44) belong to the blue region.

Here  $i$  runs over all components of the behavior  $\vec{P}(ab|xy)$  seen as a vector in  $\mathbb{R}^8$  and  $\text{NPA}_\ell$  stands for the  $\ell^{\text{th}}$  level of the NPA hierarchy. The result of this optimization is zero iff the point is on the boundary of the NPA relaxation. Fig. III.1 shows the result of this optimization as a function of the parameters  $b_1, b_0$  in the case  $\theta = \pi/8$ . We see that all statistics outside the considered region Eq. (III.44) and its symmetric version for  $B_1 \leftrightarrow B_0$  (i.e.  $b_1 > b_0$ ) admit a decomposition.

This analysis does not allow one to conclude whether the limit points on the border of the square region (for which  $b_y = \min(2\theta, \pi - 2\theta)$ ) can be self-tested or not. The method gives only unsatisfying candidates with decomposition into a single square. In Chapter V, we provide an answer to this question, showing that these points self-test the underlying implementation but not with a single Bell expression – i.e. they are non-exposed [26, 79].

### III.4.2 . Insight on geometrical properties of the quantum set

The maximal quantum value of the expressions given by Eq. (III.48) enable us to self-test states and settings for which self-testing was already known to be possible with other Bell expressions. Indeed, the partially entangled states  $|\phi_\theta\rangle$  can be self-tested using the so-called tilted CHSH expressions [65, 80]

$$I_{\alpha(\theta)} = \beta_{\text{CHSH}} + \alpha(\theta)A_0 \preceq \sqrt{8 + 2\alpha^2}, \quad (\text{III.50})$$

where  $\alpha(\theta) = 2/\sqrt{1 + 2 \tan^2(2\theta)}$  for  $\theta \in (0, \pi/4]$ . The self-tested measurement settings are given by Eq. (III.40) for fixed parameters  $b_0 = -b_1 = b_\theta$  verifying  $\tan(b_\theta) = \sin(2\theta)$ . Notice that  $b_\theta < 2\theta$  and thus the correlator points achieved with the settings maximally violating the tilted CHSH inequality can also be self-tested using  $\beta_{\theta, b_\theta, -b_\theta}$ .

Since these two expressions differ, the correlator point corresponding to

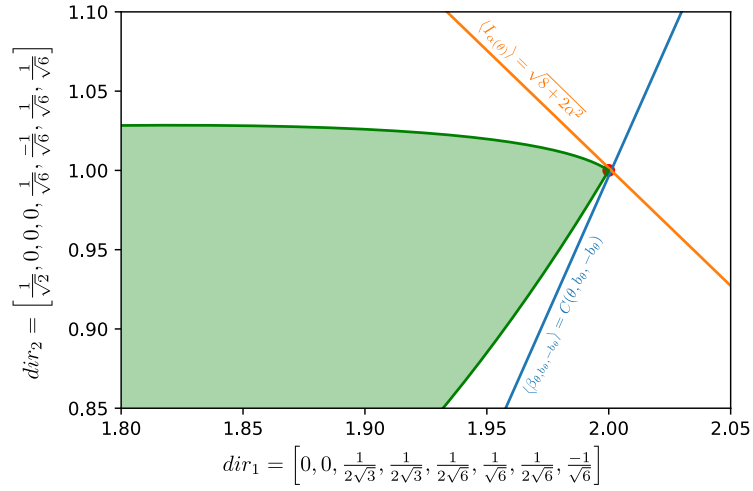


Figure III.2: The green area shows the upper bound on the quantum set given by the NPA hierarchy at level 1+AB in the slice specified by  $dir_1$  and  $dir_2$ . The directions are specified by  $dir_x = [\langle A_0 \rangle, \langle A_1 \rangle, \langle B_0 \rangle, \langle B_1 \rangle, \langle A_0 B_0 \rangle, \langle A_1 B_0 \rangle, \langle A_0 B_1 \rangle, \langle A_1 B_1 \rangle]$ . The red point is the quantum point achieved by the tilted CHSH settings for  $\theta = \pi/8$ . The orange line correspond to the tilted CHSH inequality at this point and the blue line correspond to our new inequality. The quantum set cannot go beyond these two lines.

one tilted CHSH expression can be self-tested using two different Bell expressions. In fact, it can be self-tested using the maximal quantum value of any convex combination of the tilted CHSH expression  $I_{\alpha(\theta)}$  and the new Bell expression  $\beta_{\theta, b_{\theta}, -b_{\theta}}$  we presented. Geometrically speaking, it means that this quantum point admits a one parameter family of exposing hyperplanes and that the boundary of the quantum set admits nonlocal angular point, see Fig. III.2. This led us to look into the set of inequalities that can be saturated by a given point on the border of  $\mathcal{Q}$ .





## IV – Extremal Tsirelson inequalities

The dual of the quantum set encodes the Tsirelson bounds of all possible Bell expressions [11, 81]. Describing it is therefore as challenging as finding the quantum bound of an arbitrary Bell expression, but also as important, since quantum bounds play a key role in many quantum information results [10, 14, 82]. The duality perspective already brought insight into the local and no-signaling sets, which are the two other major sets of interest in Bell-type experiments. Namely, for Bell scenarios with binary inputs and outputs it was shown that the local set, describing statistical distributions compatible with a local hidden variable model, is dual to the no-signaling set, which includes all behaviors compatible with the principles of special relativity [20]. In other words, every extremal (or ‘tight’) Bell inequality in this scenario is in one-to-one correspondence with an extremal point of the no-signaling polytope.

Unlike its local and no-signaling counterparts, the quantum set is not a polytope and little is known about its dual picture. A first result concerns the subset of vanishing marginal statistics in the CHSH scenario, corresponding to a subspace  $\mathcal{Q}_c$  of dimension 4. It was recently shown that this subspace is self-dual, i.e.  $\mathcal{Q}_c \cong \mathcal{Q}_c^*$  [20, 83]. This striking property sets the quantum set apart from both the local and the no-signaling sets. In fact, the analytical descriptions of  $\mathcal{Q}_c$  and  $\mathcal{Q}_c^*$  are fully known within this subspace: a first explicit description of the quantum set in the subspace of vanishing marginals was provided in [11, 84, 85]; see also [83, 86, 87] for explicit descriptions of its (isomorphic) dual.

Apart from this strong result for a special case, surprisingly little seems to be known about the dual quantum set  $\mathcal{Q}^*$ . Numerical studies suggested, though, that the Tsirelson point, which is the unique quantum realization maximally violating the CHSH inequality, may maximize more than one Bell expression [26]. This may be a key towards understanding whether  $\mathcal{Q}$  and  $\mathcal{Q}^*$  are being complementary but really different objects.

Here, we study the dual of the quantum set in the full 8-dimensional space with an approach consisting of finding all Bell expressions maximized by a given quantum point. Specifically, we determine analytically all elements of the dual which are related to the Tsirelson point, the unique quantum point maximally violating the Clauser-Horne-Shimony-Holt (CHSH) inequality [9]. This allows us to describe for the first time extremal points and a complete face of the dual quantum set  $\mathcal{Q}^*$ . In turn, this provides a tight first order description of the quantum set around this maximally nonlocal point.

## IV.1 - Orthogonal face of points of $\mathcal{Q}$

### IV.1.1 . More elements of convex geometry

For all this section,  $\mathcal{K} \subset \mathbb{R}^n$  denotes an arbitrary convex set. First, let's generalize the notion of extremal points to an arbitrary dimension: a subset  $F \subset \mathcal{K}$  is a *face* of  $\mathcal{K}$ , denoted  $F \triangleleft \mathcal{K}$ , iff:

$$\forall y, z \in \mathcal{K}, \lambda \in (0, 1), \lambda y + (1 - \lambda)z \in F \implies y, z \in F \quad (\text{IV.1})$$

Note that a face  $F \triangleleft \mathcal{K}$  is a convex set. The *face dimension* of a face  $F$ , denoted  $d_F$ , is the affine dimension of  $F$ . For example, the subset of local points reaching a CHSH value of 2 forms a face  $F_C$  of the local polytope (as a set of correlations), containing 8 deterministic points, of maximal face dimension 7. Extremal points of  $\mathcal{K}$  are exactly the faces of dimension 0.

Given a face  $F \triangleleft \mathcal{K}$ , one can then introduce the *orthogonal face* of  $F$ , given by

$$F^\perp = \{f \in \mathcal{K}^* : \forall x \in F, f \cdot x = 1\}. \quad (\text{IV.2})$$

The set  $F^\perp$  is a face of the convex dual  $\mathcal{K}^*$ . We call *orthogonal dimension* of  $F$ , denoted  $d_F^\perp$ , the face dimension of  $F^\perp$ . To any face  $F$  it is thus possible to associate a unique *dimension pair*: the couple  $(d_F, d_F^\perp)$ . In nonlocality, the orthogonal face encodes the set of all Bell expressions maximized by all points of the face. For example, all local points in  $F_C$  maximize the CHSH expression  $\vec{\beta}_{\text{CHSH}}/2$  and no other inequality is saturated simultaneously by all those 8 deterministic points: we have  $F_C^\perp = \{\vec{\beta}_{\text{CHSH}}/2\}$  and its dimension pair is  $(7, 0)$ . Conversely, one could notice that the CHSH inequality is maximized only by those eight extremal points and as such identifies the face  $F_C$ . In that sense, one can generalize the notion of exposed points to arbitrary faces: we say that a face  $F \triangleleft \mathcal{K}$  is *exposed* if there exists an element  $f \in F^\perp$  such that

$$\forall x \in \mathcal{K}, f \cdot x = 1 \implies x \in F.$$

Note that whenever  $F$  is exposed, it verifies  $d_F = d_{F^\perp}^\perp$ . In this case, we refer to  $d_F^\perp$  as the *dual dimension* of  $F$  that we denote  $d_F^*$ .

Finally, the study of the orthogonal face  $F^\perp$  of any face  $F \triangleleft \mathcal{K}$  can be reduced to the study of the extremal points  $\vec{P} \in \mathcal{K}$  contained in  $F$ . Indeed, any face is the convex hull of the extremal points it contains:  $F = \text{Conv}(\text{Ext}(\mathcal{K}) \cap F)$ . Therefore, one can notice that

$$F^\perp = \bigcap_{\vec{P} \in \text{Ext}(\mathcal{K}) \cap F} \{\vec{P}\}^\perp, \quad (\text{IV.3})$$

reducing the general analysis of the orthogonal faces to the ones of extremal points only<sup>1</sup>.

<sup>1</sup>This however requires having knowledge of the set of extremal points  $\text{Ext}(\mathcal{K})$ .

Let  $\mathcal{K}, \mathcal{K}'$  be two convex sets over  $\mathbb{R}^n$ . We say that  $\mathcal{K}$  and  $\mathcal{K}'$  are *isomorphic* convex sets iff there exists a linear isomorphism  $U$  of  $\mathbb{R}^n$  such that  $U(\mathcal{K}) = \mathcal{K}'$ . If two sets are isomorphic, then their duals are isomorphic too. Moreover, every face of  $F \triangleleft \mathcal{K}$  is isomorphic to a face  $U(F) \triangleleft \mathcal{K}'$  of equal dimension pair. As such, all the notion that we introduced previously are interesting as they allow for a classification of convex sets through the notion of isomorphism but also for a classification of the different type of faces of a given set.

To the physical problem of identifying all Bell expressions maximized by a given set of points, we associated the mathematical idea of computing the orthogonal face. With it comes the tool that is the dimension pair as it allow to properly characterize some properties of this set of expressions, independently of any linear isomorphic transformation that could be done (including relabeling of the correlators for example).

#### IV.1.2. General approach for deriving orthogonal faces in Bell scenarios

In a Bell scenario, even tough the set of extremal points of the quantum set is unknown, we know that each admits a quantum realization. Thus, we now focus on a given realization, independently of whether the corresponding correlator vector is extremal, and aim to compute the set of all Bell expressions that it can maximize. The state and measurements are fixed, which allows us to further develop some idea and tools that are generic to this task.

Let's consider a given realization  $(|\psi\rangle, \{\Pi_{a,x}^{(j)}\}_{a,x,j})$  and its associated correlations  $\vec{P}$ . For a given choice of measurements we introduce the measurement vector  $\vec{M}$  which is the set of all measurements that are physically measured:

$$\vec{M} = \{\Pi_{a_1, x_1}^{(1)} \dots \Pi_{a_n, x_n}^{(n)}\}_{\vec{a}, \vec{x}}. \quad (\text{IV.4})$$

For any given Bell expression  $\vec{\beta} \in \mathcal{Q}^*$ , one can then construct the Bell operator associated to this measurement choice as  $\hat{S} = \vec{\beta} \cdot \vec{M}$ , which is an hermitian operator. For any state  $|\xi\rangle$  of identical local dimensions, the correlations for the same measurement choice are given by  $\vec{P}' = \langle \xi | \vec{M} | \xi \rangle$  and the value of the Bell expression on this point is

$$\vec{\beta} \cdot \vec{P}' = \langle \xi | \hat{S} | \xi \rangle. \quad (\text{IV.5})$$

As such, if the point  $\vec{P}$  is to give the maximal quantum value of  $\vec{\beta}$ , then the state  $|\psi\rangle$  must be an eigenstate of  $\hat{S}$  (of maximal eigenvalue). This implies that for all vector  $|\xi\rangle$  orthogonal to  $|\psi\rangle$ , we have  $\langle \xi | \hat{S} | \psi \rangle = \lambda \langle \xi | \psi \rangle = 0$ . Since  $\langle \xi | \hat{S} | \xi \rangle = \vec{\beta} \cdot \langle \xi | \vec{M} | \psi \rangle$ , we obtain:

$$\vec{\beta} \cdot \vec{T}_{|\xi\rangle} = 0 \quad (\text{IV.6})$$

where we denoted  $\vec{T}_{|\xi\rangle} = \langle \xi | \vec{M} | \psi \rangle$  for any  $|\xi\rangle$  orthogonal to  $|\psi\rangle$ . Note that not all orthogonal vectors to  $|\psi\rangle$  need to be considered but only a finite number of them constituting a basis of the orthogonal space  $|\psi\rangle^\perp$ .

Suppose now that the measurements can be parameterized as functions of an arbitrary number  $m$  of real parameters  $\Pi_{a,x}^{(j)}(r_1, \dots, r_m)$ , and that our measurements of choice correspond to  $\vec{r} = 0$ . This is often the case, as for example one could rotate continuously the angle of the measurement basis. When this is the case, the correlations can also be expressed locally as a function  $\vec{P}(r_1, \dots, r_m)$ . A necessary condition to get a maximal violation is that for any small variation of the parameters  $r_i$ , the value of the Bell expression should be non-increasing. At first order, this gives

$$\forall i, \vec{\beta} \cdot \left. \frac{\partial \vec{P}}{\partial r_i} \right|_{\vec{r}=0} = 0. \quad (\text{IV.7})$$

Finally, we obtained a set of necessary linear conditions for a Bell expression  $\vec{\beta}$  to be maximized by our correlations of interest  $\vec{P}$ . They can be summarized in the following way:

$$\vec{\beta} \in V^\perp, \quad \text{where } V = \text{Vect} \left\langle \{ \vec{T}_{|\xi\rangle} | \langle \xi | \psi \rangle = 0 \} \cup \left\{ \frac{\partial \vec{P}}{\partial r_i} \right\}_i \right\rangle. \quad (\text{IV.8})$$

Interestingly enough, this proves that the orthogonal face  $\{\vec{P}\}^\perp$  is included in the orthogonal of a particular vector space. This allows to reduce the range of Bell expressions to a linear subspace, and thus upper bounds the face dimension of  $\vec{P}$  to  $\dim V$ . While these conditions do not ensure that the Bell expressions are globally maximized by  $\vec{P}$ , they are way easier to verify than the quadratic constraints of computing Tsirelson bounds. These conditions can also be used for solving of optimization problems [26, 79].

Note that we only restricted our analysis to the study of orthogonal faces of extremal points. However, since any face can be written as the convex hull of the extremal points it contains, its orthogonal face would be the intersection of the orthogonal faces of these extremal points.

## IV.2 - Orthogonal faces in the CHSH scenario

In the CHSH scenario, the search for extremal points of the quantum set  $\mathcal{Q}$  can be reduced to correlations admitting a pure state realization on real Hilbert spaces of local dimension two [88]. This reduces the characterization of orthogonal faces to knowing whether such realizations give rise to extremal correlators (see Chapter V) and studying the orthogonal face of each of these extremal points. In this section, we look at the latter, by applying the method of the previous section in three steps: first, we parameterize the set of candidate extremal correlators; second, we ask for Bell expressions to verify the eigenvector conditions ( $\vec{\beta} \cdot \vec{T} = 0$ ); third, we look for the non-increasing expressions under small variations of the realization parameters.

First, candidate extremal correlators admit realizations that can be parameterized, up to local unitaries, with a partially entangled two qubit state and real unitary measurements as

$$\text{state: } |\phi_\theta\rangle = c_\theta |00\rangle + s_\theta |11\rangle, \quad \theta \in [0, \pi/4], \quad (\text{IV.9a})$$

$$\text{measurements: } A_x = c_{a_x} \hat{Z}_A + s_{a_x} \hat{X}_A, \quad a_x \in [0, 2\pi), \quad (\text{IV.9b})$$

$$B_y = c_{b_y} \hat{Z}_B + s_{b_y} \hat{X}_B, \quad b_y \in [0, 2\pi), \quad (\text{IV.9c})$$

where operators  $\hat{Z}_{A(B)}$ ,  $\hat{X}_{A(B)}$  denote the Pauli  $z$  and  $x$  on Alice and Bob respectively. Note that this implementation only gives local probabilities whenever  $\theta = 0$ . Therefore, in all the following, we assume  $\theta > 0$ . This implementation gives the following probability distribution:

$$\vec{P}_{\theta, a_x, b_y} = \frac{1}{\begin{array}{c|c} c_{2\theta}c_{a_0} & c_{2\theta}c_{b_0} \\ \hline c_{2\theta}c_{a_1} & c_{a_x}c_{b_y} + s_{2\theta}s_{a_x}s_{b_y} \end{array}}, \quad \theta, a_x, b_y \in \mathbb{R} \quad (\text{IV.10})$$

Note that it is not granted that such a point is extremal in the set  $\mathcal{Q}$  (see Chapter V for a detailed discussion on this topic). We are now looking to describe the orthogonal face of such a point  $\vec{P}_{\theta, a_x, b_y}$ , i.e. the set of all Bell expressions with quantum bound 1 reached by this realization. In general, all possible Bell expressions can be parameterized by eight real coefficients  $a_x, b_y, c_{xy}$  for  $x, y \in \{0, 1\}$  and be written as:

$$\vec{\beta} = \{a_0, a_1, b_0, b_1, c_{00}, c_{10}, c_{01}, c_{11}\}. \quad (\text{IV.11})$$

Second, in this specific case the Bell operator induced by such a Bell expression and the considered realization Eq. (IV.9) is

$$\begin{aligned} \hat{S} = & p_1 Z_A + p_2 X_A + p_3 Z_B + p_4 X_B \\ & + p_5 Z_A Z_B + p_6 X_A X_B + p_7 Z_A X_B + p_8 X_A Z_B, \end{aligned} \quad (\text{IV.12})$$

replacing all unknown measurements  $A_x, B_y$  by their quantum implementation, and where parameters  $p_r$  are linear combinations of parameters  $a_x, b_y, c_{xy}$ . One can then find three vectors which form a basis of the orthogonal of  $|\phi_\theta\rangle$ , for example  $|\xi_1\rangle = -s_\theta |00\rangle + c_\theta |11\rangle$ ,  $|\xi_2\rangle = |01\rangle$  and  $|\xi_3\rangle = |10\rangle$ . Together with Eq. (IV.12), one can compute the vectors  $\vec{T}_i = \langle \xi_i | \hat{S} | \phi_\theta \rangle$  in terms of the parameters  $p_i$ . Our analysis show that conditions  $\vec{\beta} \cdot \vec{T}_i = 0$  allows one to reduce the range of Bell expressions to the ones for which

$$\hat{S} = 1 + \sum_{k=0}^4 p_k \hat{N}_k \quad (\text{IV.13})$$

where the  $\hat{N}_i$  forms a basis of nullifiers of  $|\phi_\theta\rangle$  [65]:

$$\begin{aligned}
\hat{N}_0 &= \hat{Z}_A - \hat{Z}_B, \\
\hat{N}_1 &= \mathbb{1} - \hat{Z}_A \hat{Z}_B, \\
\hat{N}_2 &= \hat{X}_A \hat{Z}_B + \hat{Z}_A \hat{X}_B - \frac{1 - s_{2\theta}}{c_{2\theta}} (\hat{X}_A + \hat{X}_B), \\
\hat{N}_3 &= (1 + s_{2\theta})(\hat{X}_A - \hat{X}_B) - c_{2\theta}(\hat{X}_A \hat{Z}_B - \hat{Z}_A \hat{X}_B), \\
\hat{N}_4 &= \mathbb{1} - s_{2\theta} \hat{X}_A \hat{X}_B - c_{2\theta} \hat{Z}_B.
\end{aligned} \tag{IV.14}$$

Taking this into account, we can now rewrite our candidate Bell expressions by inverting the relation Eq. (IV.9), replacing the operators  $\hat{Z}_{A(B)}$ ,  $\hat{X}_{A(B)}$  by the measurement operators  $\hat{A}_x$ ,  $\hat{B}_y$ , and one-to-one lifting to formal polynomials.

Notice that since for all  $i$ , we have  $\hat{N}_i |\phi_\theta\rangle = 0$  and that we want that the realization of interest verify  $1 = \vec{\beta} \cdot \vec{P} = \langle \phi_\theta | \hat{S} | \phi_\theta \rangle$ , we have an additional linear constrain

$$1 + p_1 + p_4 = 0. \tag{IV.15}$$

Third, we can now use the fact that small variations around the point of interest should not increase the value of the Bell expression. Our analysis shows that it suffices to consider variations of one Alice and one Bob measurement only. This condition gives a set of two linear equations:

$$0 = \vec{\beta} \cdot \frac{\partial \vec{P}_{\theta, a_x, b_y}}{\partial a_0} = \vec{\beta} \cdot \frac{\partial \vec{P}_{\theta, a_x, b_y}}{\partial b_0} \tag{IV.16}$$

which reduce to

$$\begin{aligned}
-p_0 c_{2\theta} s_{a_0} s_{a_1} + p_1 s_{a_0} s_{a_1} - \left(-p_3 - \frac{p_2}{c_{2\theta}}\right) c_{2\theta} s_{2\theta} s_{a_0+a_1} + p_4 s_{2\theta}^2 c_{a_0} c_{a_1} &= 0, \\
p_0 c_{2\theta} s_{b_0} s_{b_1} + p_1 s_{b_0} s_{b_1} - \left(p_3 - \frac{p_2}{c_{2\theta}}\right) c_{2\theta} s_{2\theta} s_{b_0+b_1} + p_4 (c_{2\theta}^2 s_{b_0} s_{b_1} + s_{2\theta}^2 c_{b_0} c_{b_1}) &= 0.
\end{aligned} \tag{IV.17}$$

The search space for the Bell expressions is thus reduced to the ones parameterized by Eq. (IV.13) verifying both Eq. (IV.15) and Eq. (IV.17). One can show that for every nonlocal cases, this linear system of equation is of rank 3. As such, the search for Bell expressions maximized by  $\vec{P}_{\theta, a_x, b_y}$  can be reduced to an affine plane of the form:

$$\vec{\beta} = \vec{\beta}_0 + \lambda_1 \vec{\beta}_1 + \lambda_2 \vec{\beta}_2 \tag{IV.18}$$

where  $\lambda_1, \lambda_2 \in \mathbb{R}$  and expressions  $\vec{\beta}_i$  verify  $\vec{\beta}_i \cdot \vec{P}_{\theta, a_x, b_y} = \delta_{i0}$ . In particular, this means that in the CHSH scenario, the orthogonal dimension of every nonlocal extremal point is upper bounded by 2. This gives an interesting starting point to study the relationship between  $\mathcal{Q}$  and  $\mathcal{Q}^*$ .

### IV.3 - Example of the Tsirelson point

We now focus on the specific case of the Tsirelson point. This point (introduced in Eq. (I.18)) is the only one maximally violating the CHSH expression (reaching the value  $2\sqrt{2}$ ). In the first chapter we highlighted that it also self-tests a unique two qubit realization of the form Eq. (IV.9) for parameters  $\theta = \pi/4$ ,  $a_0 = 0$ ,  $a_1 = \pi/2$  and  $b_y = (-1)^y \pi/4$ . In this case, Eq. (IV.15) and Eq. (IV.17) reduce to:

$$\begin{cases} 1 + p_1 + p_4 = 0, \\ p_2 = 0, \\ -p_1 + p_4 = 0 \end{cases} \quad (\text{IV.19})$$

The search space for the Bell expressions is thus reduced to

$$\beta_{r_0, r_1} = \frac{\beta_{\text{CHSH}}}{2\sqrt{2}} + r_0 \left( \frac{A_0 + A_1}{\sqrt{2}} - B_0 \right) + r_1 \left( \frac{A_0 - A_1}{\sqrt{2}} - B_1 \right), \quad (\text{IV.20})$$

in the formal polynomial formalism, where  $r_0, r_1 \in \mathbb{R}$  and  $\beta_{\text{CHSH}} = (A_0 + A_1)B_0 + (A_0 - A_1)B_1$ . Further order perturbations can be considered to reduce the range of the parameters  $r_0, r_1$ , but it turns out to be more restrictive at this stage to eliminate parameters based on the local bound of the Bell expressions. Indeed, any  $\beta_{r_0, r_1}$  with a local bound larger than 1 also admits a quantum value larger than 1 (and hence larger than the value obtained on  $\vec{P}_T$ ).

#### IV.3.1 . Local bounds

Since the convex combination of two polynomials with a local bound smaller than one also has a local bound smaller than one, the set of expressions  $\beta_{r_0, r_1}$  with a local bound smaller than 1 forms a convex region of the  $r_0, r_1$  plane. Furthermore, the local maxima of a Bell expression is reached at one of the 16 extremal points of the local polytope. These points are given by

$$\vec{L}_{ijkl} = \frac{1}{k} \begin{array}{c|c|c} i & & j \\ \hline k & ik & jk \\ \hline l & il & jl \end{array}, \quad i, j, k, l \in \{-1, 1\}. \quad (\text{IV.21})$$

The convex region of expressions of the form Eq. (IV.20) with a local maxima smaller than one is thus given by all points  $(r_0, r_1)$  satisfying the conditions  $\beta_{r_0, r_1} \cdot \vec{L}_{ijkl} \leq 1$ . The intersection of these half planes defines a polytope, namely a regular octagon, whose eight summit are given by (see Fig. IV.1)

$$\left\{ \left( 1 - \frac{1}{\sqrt{2}} \right) R_{\frac{\pi}{4}}^k(1, 0), k \in \{0, \dots, 7\} \right\}, \quad (\text{IV.22})$$

where  $R_{\frac{\pi}{4}}$  is the rotation of angle  $\pi/4$  in the  $(r_0, r_1)$  plane. Any Bell expression outside this octagon has a local bound larger than 1, and thus is not maximized by  $\vec{P}_T$ .



### IV.3.2 . Quantum bounds

Having excluded a range of Bell expressions  $\beta_{r_0, r_1}$  from their local bound, we need to compute the Tsirelson bound of the expressions inside the octagon. To do so, we use the method introduced in Section III.2. Let us remind that one needs to find a positive definite matrix  $W \succeq 0$  such that  $1 - S = \vec{N}^\dagger \cdot W \cdot \vec{N}$  where  $\vec{N}$  is a generating sequence of the set of polynomials which realization nullifies the state  $|\phi^+\rangle$ . One can consider different relaxations levels  $\mathcal{T}$  of the algebra of formal polynomials. The first order relaxation  $\mathcal{T}_{1+A+B} = \{1, A_0, A_1, B_0, B_1\}$  only gives a certificate for the CHSH expression. The relaxation at the almost quantum level [89],  $\mathcal{T}_{1+A+B+AB} = \mathcal{T}_1 \cup \{A_x B_y, x, y \in \{0, 1\}\}$  can also be computed numerically and gives a certificate for a disk in the  $(r_0, r_1)$  plane of center  $(0, 0)$  and radius  $\frac{1}{4\sqrt{2}}$ . The next relaxation considered here is given by

$$\mathcal{T}_{1+A+B+AB+ABB'} = \mathcal{T}_{1+AB} \cup \{A_x B_y B_{y'}, y \neq y'\}. \quad (\text{IV.23})$$

We can show analytically that a certificate  $1 - \beta_{(1-\frac{1}{\sqrt{2}}, 0)} = \vec{N}^\dagger W_3 \vec{N}$  can be found for the expression of coordinate  $(r_0, r_1) = (1 - \frac{1}{\sqrt{2}}, 0)$  at this level of relaxation:

$$\vec{N} = \begin{pmatrix} \frac{A_0+A_1}{\sqrt{2}} - B_0 \\ 1 - \frac{A_0+A_1}{\sqrt{2}} B_0 \\ B_0 \left(1 - \frac{A_0-A_1}{\sqrt{2}} B_1\right) \\ \frac{A_0-A_1}{\sqrt{2}} - B_1 \\ B_1 \left(1 - \frac{A_0+A_1}{\sqrt{2}} B_0\right) \\ \frac{A_0+A_1}{\sqrt{2}} B_1 + \frac{A_0-A_1}{\sqrt{2}} B_0 \end{pmatrix}, \quad W_3 = \frac{1}{16} \begin{pmatrix} \sqrt{2} & -2s & -s & & & \\ -2s & 2s & 0 & & & \\ -s & 0 & \sqrt{2} & & & \\ & & & 2 & 0 & s \\ & & & 0 & \sqrt{2}s & s \\ & & & s & s & s \end{pmatrix}, \quad (\text{IV.24})$$

where  $s = 2 - \sqrt{2}$  and  $W_3 \succeq 0$ . This ensures that the Bell expression

$$\beta_T = \frac{\beta_{\text{CHSH}}}{2\sqrt{2}} + \left(1 - \frac{1}{\sqrt{2}}\right) \left(\frac{A_0 + A_1}{\sqrt{2}} - B_0\right) \quad (\text{IV.25})$$

is maximized by the Tsirelson point. Since we already concluded that a larger value of  $r_0$  admits a local value larger than 1, this bound for  $r_1 = 0$  is the best we could have hoped for. One can check that this expression is an extremal point of  $\mathcal{Q}^*$ , that it is exposed<sup>2</sup>, and that it is only maximized by 3 extremal points of  $\mathcal{Q}$ :  $\vec{P}_T$  and two deterministic realizations.

To analyze the rest of the octagon, we make use of some symmetries of the problem. Both the family of Bell expressions  $\beta_{r_0, r_1}$  and the set  $\mathcal{Q}$  are preserved by several discrete symmetries. One of them is described by the following action:

$$S : (r_0, r_1) \rightarrow R_{\frac{\pi}{4}}(r_0, r_1), \quad \begin{cases} A_0 \rightarrow -B_1, & A_1 \rightarrow -B_0, \\ B_0 \rightarrow -A_0, & B_1 \rightarrow A_1. \end{cases} \quad (\text{IV.26})$$

<sup>2</sup>i.e. the quantum set admits a point which only saturates this Tsirelson inequality.

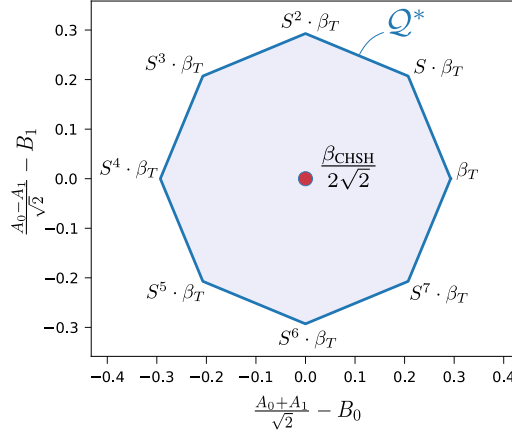


Figure IV.1: Face of  $\mathcal{Q}^*$  in the two-dimensional affine slice defined by  $\beta_{r_0, r_1}$  for real parameters  $r_0, r_1$ . The red point in the middle, the normalized CHSH expression, is non-extremal: it can be decomposed in terms of the eight summits of the octagon, which are extremal Tsirelson inequalities.

Due to this symmetry, the quantum bound of any Bell expression with parameters  $(r_0, r_1) \in \mathbb{R}^2$  can be computed by looking at the bound of the inequality with parameters rotated by  $\pi/4$ . This ensures that the quantum bounds of the eight inequalities  $S^k \cdot \beta_T$  of polar coordinates  $(1 - \frac{1}{\sqrt{2}}, k\frac{\pi}{4})$  for  $k \in \{0, \dots, 7\}$  are also one. Therefore, the octagon is exactly the convex region of quantum bound equal to 1. This completes the characterization of the slice  $\beta_{r_0, r_1}$  (see Fig. IV.1).

Interestingly, the normalized CHSH expression lies in the middle of this dual face. Therefore, it is not an extremal Tsirelson inequality. In particular, we can write it as the convex mixture

$$\beta_{\text{CHSH}} = \frac{1}{2} (\beta_T + S^4 \cdot \beta_T). \quad (\text{IV.27})$$

Note that this description is not unique because  $\beta_{\text{CHSH}}$  lies in the middle of a face of  $\mathcal{Q}^*$  of dimension 2.

From the point of view of the quantum set, this means that the Tsirelson point  $\vec{P}_T$  is an exposed extremal point of  $\mathcal{Q}$  with dimension pair  $(0, 2)$ , i.e. with a face dimension of 0 and a dual dimension of 2. Furthermore, it is exposed by all the expressions on the inside of the octagon (see Fig. IV.2). In fact, any Bell expression inside the octagon can be written as a convex combination of the CHSH expression and an expression  $\beta_b$  on the border of the octagon:  $\beta = p\beta_{\text{CHSH}}/2\sqrt{2} + (1-p)\beta_b$ , where  $p \in (0, 1]$ . If a point  $\vec{P}$  verifies  $\vec{\beta} \cdot \vec{P} = 1$ , then it implies  $\vec{\beta}_{\text{CHSH}} \cdot \vec{P} = 2\sqrt{2}$  and the self-testing result of  $\beta_{\text{CHSH}}$  implies that  $\vec{P} = \vec{P}_T$ . From the self-testing point of view, this means that any Tsirelson inequality inside the octagon self-tests the singlet state  $|\phi^+\rangle$  and measurements Eq. (I.17) associated to the Tsirelson point. As far as expressions on the border of the octagon are concerned, these are also maximized by local points and as such cannot provide a self-test of the realization.

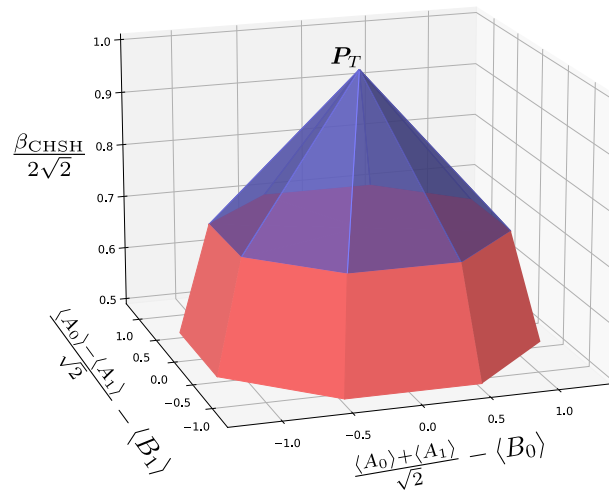


Figure IV.2: Three-dimensional projection of the local polytope (in red) and of the quantum set of correlations (red and blue). The only point reaching the z-value of 1 is the Tsirelson realization. This point lies on top of an octagonal-based pyramid whose eight facets correspond to the Bell expressions  $S^k \cdot \beta_T$  for  $k = 0, \dots, 7$ .

## V – Quantum statistics in the CHSH scenario

What are the fundamental limits of quantum theory's probabilistic predictions? Considering this problem already in the 1980s, Tsirelson was the first to obtain bounds on the quantum set [23, 90]. Several results followed, notably from Landau and Masanes [84, 85], until major progress was achieved by Navascués, Pironio and Acín (NPA) in the form of a hierarchy of semidefinite programming [13, 57]. Concretely, the hierarchy defines a family of problems of increasing complexity which approximate better and better the quantum set from the outside and guarantees convergence as the level of the hierarchy goes to infinity. At a fixed hierarchy level, this technique allows deriving necessary conditions for the quantum set [91], thus excluding that some behaviors admit a quantum representation. However, since the NPA technique can generally not guarantee that specific statistics are quantum, its implications remain elusive on the boundary of the quantum set.

Recently, fresh insight was gained on the quantum set by analytical studies which showed that it admits flat nonlocal boundaries [26, 79], as well as pointy nonlocal extremal points [86, 92]. New curved regions of the set's boundaries were also identified analytically [93] and several conjectures were formulated on the boundary of the quantum set [88, 94].

In this chapter, we consider the question of identifying the limits of the quantum set from the perspective of self-testing [24]. So far, numerous families of states have been shown to be self-testable through some of their behaviors [59, 60]. However, only the statistics obtained when measuring a maximally entangled state in the CHSH scenario have been fully characterized by self-testing [78]. These behaviors correspond to the boundary of the quantum set in this scenario with vanishing marginals, which was described earlier by Tsirelson, Landau and Masanes, see [83].

Here, we obtain all the self-tests in the CHSH scenario. This reveals previously unknown boundaries of the quantum set. In turn, it allows us to identify all extremal points and their corresponding quantum realizations, thus providing a complete description of the quantum set in this minimal scenario.

### V.1 - Restriction to a fixed parameter range

Since  $\mathcal{Q}$  is convex, it is fully described as the convex hull of its extremal points:  $\mathcal{Q} = \text{Conv}(\text{Ext}(\mathcal{Q}))$ . The subset of extremal points in  $\mathcal{Q}$  has been many times restricted using different arguments. First, since the local Hilbert space

dimensions are not fixed, using Naimark's dilation theorem, one can always restrict to realizations involving pure states and unitary measurements. Second, using Jordan's lemma, the search for extremal points can be limited to realizations of local Hilbert space dimension 2 [95]. Last, more recent results show that it suffices to consider realizations with real Hilbert spaces [88]. As such,  $\text{Ext}(\mathcal{Q}) \subset \mathcal{Q}_2$  where  $\mathcal{Q}_2$  is included in the set of points which can be achieved by measuring a partially entangled two qubit state with real unitary measurements, i.e. realized by:

$$|\phi_\theta\rangle = \cos\theta |00\rangle + \sin\theta |11\rangle, \quad (\text{V.1a})$$

$$A_x = \cos a_x \sigma_z + \sin a_x \sigma_x, \quad (\text{V.1b})$$

$$B_y = \cos b_y \sigma_z + \sin b_y \sigma_x. \quad (\text{V.1c})$$

This subset of realizations thus stands out as a set of particular interest.

The set  $\mathcal{Q}$  exhibits intrinsic symmetries due to how it is constructed: it should be symmetric under relabelling of inputs and/or outputs, and under exchange of parties. In particular, the nature of a point (extremal or not) is unchanged by such symmetries. These can be translated to transformations on the measurements performed by Alice and Bob. For a realization Eq. (V.1) of a point in  $\mathcal{Q}_2$ , the symmetries of  $\mathcal{Q}$  render to involutions on the parameters  $a_x, b_y$ . In particular, one can restrict the analysis of the nature of points in  $\mathcal{Q}_2$  to the following range of parameters:

$$\theta \in [0, \pi), 0 \leq a_0 \leq b_0 \leq b_1 < \pi, a_0 \leq a_1 < \pi, \quad (\text{V.2})$$

Any realization outside this range can be uniquely transformed into a realization in this range, using the symmetries of  $\mathcal{Q}$ , and the nature of the two corresponding points will be the same.

Note that whenever the quantum realization involves a separable state, then the corresponding point lies in the local set. In particular, this is the case for any point in  $\mathcal{Q}_2$  involving a state with entanglement parameter  $\theta \cong 0[\pi/2]$ . The extremal points of the local polytope are known and correspond to the 16 deterministic strategies, for which  $\langle A_x \rangle = a$ ,  $\langle B_y \rangle = b$  and  $\langle A_x B_y \rangle = ab$ , for  $a, b \in \{-1, 1\}$ . Since these are also extremal in the non-signaling polytope and since  $\mathcal{Q} \subset \mathcal{N}$ , they are extremal in  $\mathcal{Q}$ . As such, when considering qubit realizations, we consider that they are achieved with an entangled state, i.e.  $\theta \not\cong 0[\pi/2]$ .

## V.2 - Steering of quantum realizations

In order to characterize the realization of local dimension 2, we consider a non-linear map  $T_\theta : \mathcal{H}_A \rightarrow \mathcal{H}_A$  which describes the steering of a vector  $|u\rangle$

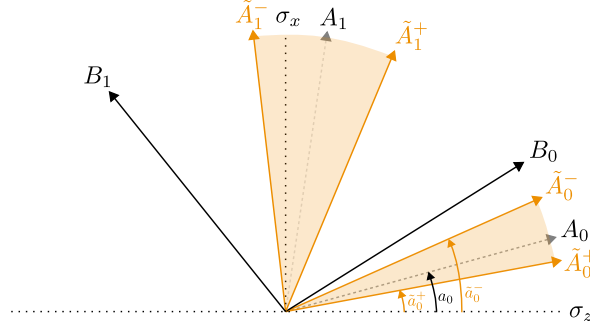


Figure V.1: Action of the steering transformation on a realization involving two measurements for each party. When the entanglement parameter  $\theta$  is in  $(0, \pi/4)$  and Alice's measurements are in the  $(\sigma_z, \sigma_x)$  upper-plane, the steered realization involves four new measurements  $\tilde{A}_x^a$ , with respective angles  $\tilde{a}_x^a$  to  $\sigma_z$  in the same plane.

in Alice's Hilbert space through the state  $|\phi_\theta\rangle$ :

$$T_\theta : |u\rangle \mapsto \frac{\sqrt{2}\langle\phi_\theta|u\rangle|\phi^+\rangle}{\|\langle\phi_\theta|u\rangle\|_2}, \quad (\text{V.3})$$

where  $|\phi^+\rangle := |\phi_{\pi/4}\rangle$  is the maximally entangled two qubit state. This transformation correspond to the identity if the initial state is  $|\phi^+\rangle$ . If the initial state  $|u\rangle$  is normalized, then the image vector  $T_\theta(|u\rangle)$  also is. One can extend the action of this steering function to the set of projectors acting on Alice's Hilbert space: for any  $|u\rangle\langle u|$ , the operator  $|T_\theta(|u\rangle)\rangle\langle T_\theta(|u\rangle)|$  is itself a unit projector

However, the action of the steering transformation does not preserve orthogonality. As such, it cannot be directly extended to unitary measurements. One way to bypass this issue is to allow one to double the number of measurements on Alice's side. Indeed, for any unitary measurement  $A_x$  on Alice's Hilbert space, both  $\Pi_{a,x} := (\mathbb{1} + aA_x)/2$ , for  $a \in \{-1, 1\}$ , are projectors on which one can apply steering. Even though the image projectors won't sum to the identity, one can still define a pair of new unitary measurements  $\tilde{A}_x^a = a(2T_\theta[\Pi_{a,x}] - \mathbb{1})$ . Note that if the initial measurement has an angle  $a_x \in [0, \pi)$  with respect to  $\sigma_z$  in the  $(\sigma_z, \sigma_x)$ -plane, then the modified measurement still lie on this plane, but with modified angles  $\tilde{a}_x^a \in [0, \pi]$  with respect to  $\sigma_z$  (see Fig. V.1), where:

$$\tilde{a}_x^a = 2 \arctan\left(\tan\left(\frac{a_x}{2}\right) \tan(\theta)^a\right). \quad (\text{V.4})$$

The average value of these new operators on the maximally entangled state can be expressed as a non-linear transformation of the initial vector of correlators:

$$[\tilde{A}_x^a B_y] := \langle\phi^+|\tilde{A}_x^a B_y|\phi^+\rangle = \frac{\langle A_x B_y\rangle + (-1)^a \langle B_y\rangle}{1 + (-1)^a \langle A_x\rangle}. \quad (\text{V.5})$$

As such, upon a non-linear transformation  $T_\theta$ , the original correlation vector obtained with a realization of local dimension two can be interpreted as correlators of a quantum point realized by the state  $|\phi^+\rangle$ , four measurements for Alice and two for Bob:

$$\begin{array}{c|c|c}
\langle A_0 \rangle = c_{2\theta} c_{a_0} & \langle B_0 \rangle = c_{2\theta} c_{b_0} & \langle B_1 \rangle = c_{2\theta} c_{b_1} \\
\langle A_1 \rangle = c_{2\theta} c_{a_1} & \langle A_x B_y \rangle = c_{a_x} c_{b_y} + s_{2\theta} s_{a_x} s_{b_y} & \\
\hline
& & \xrightarrow{T_\theta} \\
\hline
& & \begin{array}{c|c}
0 & 0 \\
\hline
0 & [\tilde{A}_x^a B_y] = c_{\tilde{a}_x^a - b_y} \\
0 & \\
0 & 
\end{array}
\end{array} \quad (\text{V.6})$$

Note that all marginals of this new quantum point are equal to zero as it is the case whenever measuring a maximally entangled state. Therefore, this new point can itself be embedded in an eight dimensional space.

Since the new extended statistics (with 4 settings for Alice) are valid quantum statistics, they must satisfy known constraints on the quantum set. In particular, for each pair  $(s, t)$  corresponding to two of Alice's new measurements  $(\tilde{A}_0^s, \tilde{A}_1^t)$ , one can use previously known characterizations of the quantum set in the subspace of zero marginals of the CHSH scenario. For example, one can use the push-out characterization [83], first introduced by Masanes [85], to make the following statement:

**Proposition 1.** - *Necessary condition for pure projective realizations of local dimension 2.*

*In the CHSH scenario, any nonlocal quantum point that admits a realization with local Hilbert spaces of dimension two, a pure state and projective measurements, verifies the following inequalities, for all  $s, t \in \{-1, 1\}$ :*

$$\begin{aligned}
-\pi &\leq -\text{asin}[\tilde{A}_0^s B_0] + \text{asin}[\tilde{A}_1^t B_0] + \text{asin}[\tilde{A}_0^s B_1] + \text{asin}[\tilde{A}_1^t B_1] \leq \pi \\
-\pi &\leq \text{asin}[\tilde{A}_0^s B_0] - \text{asin}[\tilde{A}_1^t B_0] + \text{asin}[\tilde{A}_0^s B_1] + \text{asin}[\tilde{A}_1^t B_1] \leq \pi \\
-\pi &\leq \text{asin}[\tilde{A}_0^s B_0] + \text{asin}[\tilde{A}_1^t B_0] - \text{asin}[\tilde{A}_0^s B_1] + \text{asin}[\tilde{A}_1^t B_1] \leq \pi \\
-\pi &\leq \text{asin}[\tilde{A}_0^s B_0] + \text{asin}[\tilde{A}_1^t B_0] + \text{asin}[\tilde{A}_0^s B_1] - \text{asin}[\tilde{A}_1^t B_1] \leq \pi
\end{aligned} \quad (\text{V.7})$$

where for all  $a, x, y$ :  $[\tilde{A}_x^a B_y] = \frac{\langle A_x B_y \rangle + a \langle B_y \rangle}{1 + a \langle A_x \rangle}$ .

Note that inequalities for  $(s, t) = (1, 1)$  are linear combinations of inequalities for  $(s, t) \neq (1, 1)$  and as such there are only 24 independent inequalities in the above. All these inequalities can be obtained considering only one of them and using intrinsic symmetries of the quantum set of correlations that are relabelling of inputs and outputs. Moreover, one can write 24 other independent inequalities by performing the steering transformation on Bob's measurements. Finally, in the case where some of Alice's marginals are equal to  $\pm 1$ , some of the correlators  $[\tilde{A}_x^a B_y]$  are not well-defined. This can however only happen when  $\theta \equiv 0[\pi/2]$  and thus corresponds to local points.

When the marginals are zero, the inequalities collapse to only 8 convex inequalities, corresponding to the ones identifying the boundary of the quantum set in this restricted CHSH scenario [85]. However, in all generality, the inequalities Eq. (V.7) are not preserved by convex combinations and thus cannot fully describe the set  $\mathcal{Q}$ . Unlike for the zero marginal case, some quantum points, admitting a non-qubit realization, do not satisfy all of the above inequalities.

### V.3 - Self-testing statement

Self-testing describes the fact that some points in the quantum set of correlations fully identify the underlying realization, that is a state and measurements on both parties, up to local unitary transformations and additional degrees of freedom. As such, these correlators provide a device-independent characterization of physical state and measurements [14]. The self-testing property is of particular interest in our study, as self-testing correlators are extremal correlations of the quantum set (see [26, Proposition C.1]). In the CHSH scenario with zero marginals, all extremal points self-test a realization, which always involves a maximally entangled state [83] and where Alice’s and Bob’s angles of measurements “alternate” [78], i.e. when, up to intrinsic symmetries of  $\mathcal{Q}$ , the measurement parameters verify  $0 \leq a_0 \leq b_0 \leq a_1 \leq b_1 \leq \pi$ . Outside this range, the corresponding points are on the interior of the quantum set [83]. However, we know that other correlations self-test partially entangled states and as such the extremal points of  $\mathcal{Q}$  do not only correspond to realization involving a singlet state.

In the zero marginal case, the equality case in the inequalities introduced in Eq. (V.7) can only be achieved by self-testing correlations, which identify a singlet state and real unitary measurements [78]. It is thus natural to ask whether the points saturating some of the above conditions could lead to self-testing as well. It turns out that saturating a single inequality is not sufficient. Similarly, one can find non-extremal points saturating two inequalities. However, whenever three of the conditions are met for different values of  $(s, t)$ , the fourth one is also, and in this special case, we show that the resulting statistics self-test a qubit realization.

**Theorem 1.** *Any nonlocal behavior which satisfies*

$$\text{asin}[\tilde{A}_0^s B_0] + \text{asin}[\tilde{A}_1^t B_0] - \text{asin}[\tilde{A}_0^s B_1] + \text{asin}[\tilde{A}_1^t B_1] = \pi, \quad (\text{V.8})$$

*for all  $(s, t) \in \{\pm 1\}^2$ , self-tests a quantum realization of local dimension 2.*

In particular, all realizations in the range Eq. (V.2) for which the measurement angles *fully alternates*, i.e. verify

$$0 \leq [\tilde{a}_0^s]_\pi \leq b_0 \leq [\tilde{a}_1^t]_\pi \leq b_1 < \pi \quad (\text{V.9})$$



satisfy, up to relabelling, the condition of Theorem 1. As such, these realizations are self-tested by their associated quantum point, which is therefore extremal in  $\mathcal{Q}$  [26]. Note that, conversely, satisfying Eq. (V.8) for all  $(s, t) \in \{\pm 1\}^2$  self-tests realizations that fully alternate (up to relabeling).

The proof of Theorem 1, given in [96][Appendix C], strongly relies on the steering transformation. This time, the nonlinear transformation is used to map self-testing statements on a maximally entangled state into a self-testing statement on a partially entangled one. This is made possible by strong geometrical relations between the vectors  $\tilde{A}_x^a |\phi^+\rangle$  and  $B_y |\phi^+\rangle$  issued from the steered realization when Eq. (V.8) holds.

Note that the condition of nonlocal behavior implies that the marginals cannot take the value  $\pm 1$ , which guarantees that the correlators  $[\tilde{A}_x^s B_y]$  are well-defined. Indeed, any vector with a single marginal probability equal to  $\pm 1$  would have more than two zeros of probabilities on the same line or column of the probability table, ensuring that the quantum point is local [79].

## V.4 - Non-exposed condition

Theorem 1 identifies many extremal points of the quantum set and provides self-testings for all qubit partially-entangled states with a large family of measurement settings. However, it does not say whether points which do not satisfy the equality case are extremal in  $\mathcal{Q}$ . In order to address this, we consider the complementary question of showing that realizations which do not satisfy the full alternation condition Eq. (V.9) lead to behaviors that are non-extremal. As a first step in this direction, we prove that in the absence of full alternation, the statistics are non-exposed in  $\mathcal{Q}$ , i.e. that they do not uniquely reach the Tsirelson bound of any Bell expression (see Section I.1.6). Note that since non-exposed points include both decomposable points and some extremal points, this result in itself does not allow concluding yet.

**Theorem 2.** *Consider a quantum realization with state  $|\phi_\theta\rangle$  and measurements satisfying Eq. (V.2). If the following series of inequalities does not hold:*

$$\forall s, t, 0 \leq [\tilde{a}_0^s]_\pi < b_0 < [\tilde{a}_1^t]_\pi < b_1 < \pi, \quad (\text{V.10})$$

where  $\tilde{a}_x^a = 2 \operatorname{atan}(\tan(\frac{a_x}{2}) \tan(\theta)^a)$ , and  $[\alpha]_\pi := \alpha[\pi]$ , then the corresponding point is non-exposed in  $\mathcal{Q}$ .

The proof of Theorem 2, presented in [96][Appendix D] is divided into two main parts. First, we use the method presented in Section IV.1.2 which allows us to restrict the range of expressions that can be maximized by such realizations to a 3-dimensional vector space. Second, for all remaining Bell expressions, we identify a local point, different from this initial one, which gives the same Bell value. This guarantees that the value achieved by this

quantum point for every Bell expression is also achievable by another point, and therefore that the point is non-exposed.

Note that the parameter range of  $a_x, b_y$  made in the theorem can always be reached by using the intrinsic symmetries of the quantum set, as discussed earlier, without changing the nature (non-exposed) of the corresponding points.

Finally, the modified angles  $\tilde{a}_x^a$  introduced in the theorem are, up to output relabeling, the angles in the real Pauli plane of the modified measurements obtained through steering. As such, the theorem states that if the modified angles of Alice  $\tilde{a}_x^a$  and the angles of Bob  $b_y$  do not alternate, then the corresponding points are non-exposed.

## V.5 - Characterization of $\text{Ext}(\mathcal{Q})$

Equipped with Lemmas 1 and 2, let us consider a qubit realization of the form Eqs. (V.1) and (V.2). If the measurement angles satisfy the alternating condition Eq. (V.9), then Theorem 1 ensures that the quantum realization is self-tested and therefore the point is extremal. This shows that the alternating property Eq. (V.9) is constitutive of these points: no point obtained with non-alternating settings can be obtained with other, alternating settings. Using this property together with Theorem 2 ensures that all realizations that do not verify Eq. (V.9) correspond to points on the interior of the set of non-exposed points of  $\mathcal{Q}$ . However, Straszewicz's theorem states that all extremal points are limits of exposed points [19]. This ensures that non-alternating realizations lead to non-extremal points of  $\mathcal{Q}$ . This can be summarized in the following theorem.

**Theorem 3** (Characterization of  $\text{Ext}(\mathcal{Q})$ ).

1. A nonlocal point in the CHSH scenario is extremal in  $\mathcal{Q}$  iff

$$\forall \mathbf{u} \in \{\pm 1\}^2, \sum_{x,y} \epsilon_{xy} \text{asin}[\tilde{A}_x^{\mathbf{u}_x} B_y] = \pi \quad (\text{V.11})$$

for some  $\epsilon_{xy} \in \{\pm 1\}$  such that  $\prod_{x,y} \epsilon_{xy} = -1$ .

2. A quantum realization leads to a nonlocal extremal point iff it can be mapped by local channels and relabelings to a quantum realization on the entangled state  $|\phi_\theta\rangle$  with measurements satisfying Eq. (V.2) s.t.

$$\forall (\mathbf{s}, \mathbf{t}) \in \{\pm 1\}^2, 0 \leq [\tilde{a}_0^s]_\pi \leq b_0 \leq [\tilde{a}_1^t]_\pi \leq b_1 < \pi. \quad (\text{V.12})$$

Note that the full alternance condition is equivalent whether the steering transformation is applied on Alice's measurements (as done here) or on Bob's ones. Therefore, exchanging the role of Alice and Bob in conditions Eqs. (V.11)

and (V.12), with modified angles  $\tilde{b}_y^b$  and correlators  $[A_x \tilde{B}_y^b]$ , identifies the same extremal point.

When the underlying state is  $|\phi^+\rangle$ , we have  $\tilde{a}_x^a = a_x$  for all  $a, x$ . As such, the four conditions Eq. (V.12) collapse to a single one, recovering the alternating condition of the measurement for the singlet and the extremal points of the CHSH scenario with zero marginals [83].

Together with the 8 deterministic strategies [15], which are local extremal points of  $\mathcal{Q}$ , Theorem 3 gives a complete characterization of the extremal point of the quantum set in the minimal scenario. This description implies that all nonlocal extremal points in this scenario self-test a two qubit realization.

This theorem gives us a clear geometrical understanding of the realizations leading to extremal points, as depicted in Fig. V.2. Whenever the initial measurement settings  $a_x, b_y$  do not alternate, then the corresponding point is not extremal for all possible value of  $\theta$ . However, whenever the initial measurement settings  $a_x, b_y$  alternate, the corresponding point is extremal for an entanglement parameter in  $\{\theta_{\min}, \pi/4\}$ , where  $\theta_{\min}$  correspond to the largest value of  $\theta$  for which an equation of the form  $\tilde{a}_x^a = b_y$  is satisfied, as conjectured in [88].

Note that the analytical description of the quantum set given by Theorem 3 provides new insight on its geometry. It implies that the 8-dimensional convex set is generated by a 5-dimensional sub-manifold of extremal points. Indeed, as discussed above, whenever Alice's marginals are not zero, three out of the four equations above are linearly independent. Furthermore, satisfying an equation of the form  $[\tilde{A}_x^a B_y] = \pm 1$  is equivalent to saturating a positivity inequality. As such, Theorem 2 ensures that all extremal points of  $\mathcal{Q}$  lying on the border of the non-signaling polytope  $\mathcal{N}$  are non-exposed, answering positively a conjecture made in [79].

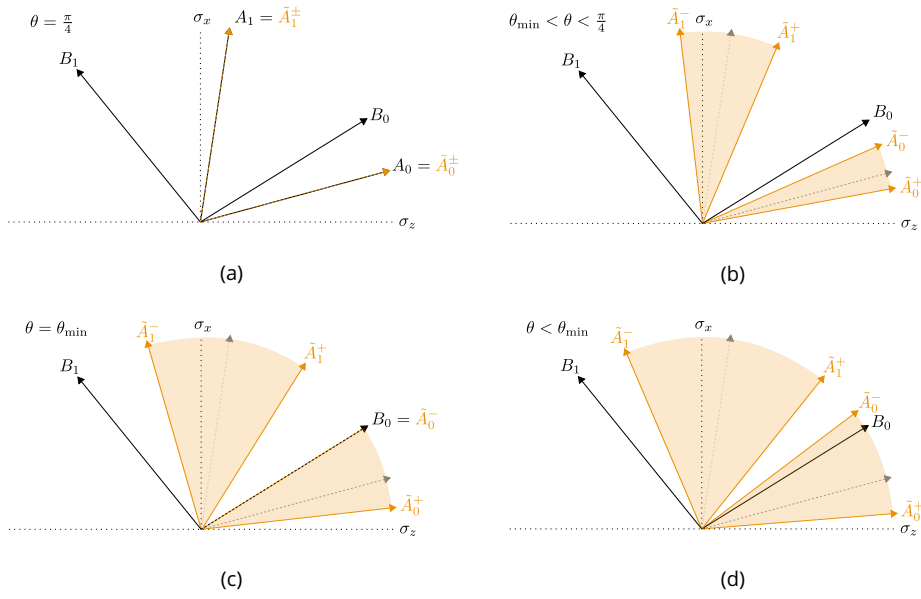


Figure V.2: Geometrical representation of the realizations leading to extremal points of the quantum set in the CHSH scenario. Up to local isometries and relabelings, these realizations correspond to measurements on a partially entangled two qubit state  $|\phi_\theta\rangle$  taking place in the  $(\sigma_z, \sigma_x)$ -plane and verifying the fully alternating condition Eq. (V.9). If the initial measurement angles alternate, i.e. verify  $0 \leq a_0 \leq b_0 \leq a_1 \leq b_1 < \pi$ , then the corresponding points are extremal for all entanglement parameters  $\theta$  in  $[\theta_{\min}, \pi/4]$ , where the threshold entanglement value is given by  $\theta_{\min} = \max\{\theta \leq \pi/4 \text{ s.t. } \tilde{a}_x^a = b_y\}$ . As such, for  $\theta = \pi/4$ , pictured in Fig. V.2a, the point is extremal. For  $\theta_{\min} < \theta < \pi/4$ , pictured in Fig. V.2b, the orange areas and black arrows still alternate, so the point is extremal. For  $\theta = \theta_{\min}$ , see Fig. V.2c, the point is still extremal but non-exposed in  $\mathcal{Q}$ . Last, for  $\theta < \theta_{\min}$ , like in Fig. V.2d, the black arrow of  $B_0$  is inside an orange area: the fully alternating property is broken, and the point admits a decomposition.



## Conclusion and Outlooks

The understanding of nonlocality and its impactful implications now allows for the development of more and more promising applications, through innovative devices and new possibilities of communications. With the rapid growth of quantum based technologies, we are faced with the challenge of certifying their proper working. As we've seen in the first chapter, Bell-like experiments in the lab are now at the point where they start to be able to certify quantum states and measurements in a device-independent way. However, many things remain to be understood on the theoretical end both to reduce the experimental requirements and make protocols more practical, and to understand the reach of such certification schemes. Moreover, many of these protocols rely on the assumption that quantum theory is a valid and complete description of nature. Our contributions in this thesis evolve mainly around two lines: finding new Bell expressions together with new self-tests for more states and more measurements, and describing the set of correlators achievable within quantum theory.

### Bell inequalities and self-testing

In this thesis, we considered the problem of constructing Bell expressions that are tailored to a generic target state in the sense that its maximal admissible quantum value can be achieved by measuring this state. We presented a solution to this problem in the form of a systematic method applicable to arbitrary quantum states, which uses a Sum of Squares of formal polynomials to define the coefficient of the Bell expression. In principle, this method is *asymptotically complete*, in the sense that every Bell expression with the desired property can be obtained by starting from a complete enough set of formal nullifiers. When the degree of the nullifiers is bounded, the method still provides *sufficient* (but not necessary) conditions for a Bell expression to be maximally violated by the target state. Therefore, in all cases, the method constructs Bell expressions with the guarantee that their maximal value is achieved by the desired state.

In addition to providing a Bell expression with the desired property, a key feature of the SOS method is that it also grants, by construction, its sum of squares. This provides a first step towards the self-testing of the quantum realization. However, clarifying when Bell expressions obtained by the SOS method exhibit the self-testing property remains an open question. Indeed, even though SOS decompositions provide a key ingredient to self-testing, complete self-testing proofs can still require substantial work [77, 97]. Finding con-

ditions under which the SOS method allows for self-testing could lead to an asymptotically complete method for self-testing target states. Possible lines of work could include using recent progress in the formulation of self-testing in more operational or algebraic ways [98, 99] or self-testing proofs relying on representation theory [100, 101]. These new approaches might help to find necessary conditions for an SOS involving a given set of nullifiers to imply self-testing.

As highlighted in chapter 2, using the SOS method, we constructed a family of Bell inequalities tailored to the maximally entangled two-qutrits state  $|\psi^3\rangle = (|00\rangle + |11\rangle + |22\rangle)/\sqrt{3}$ . We also used the method to derive a family of Bell expressions with 2 real parameters, self-testing the partially entangled state  $|\phi_\theta\rangle = \cos\theta|00\rangle + \sin\theta|11\rangle$  when Alice performs  $\sigma_z$  and  $\sigma_x$  measurements. In turn, this allowed finding new Bell expressions for realizations we already knew how to self-test. This striking fact seems to be more prevalent than one could think, as we even proved in chapter 4 that this is the case of the well-known Tsirelson point. The fact that several Bell expressions can be used to self-test the same point could help to obtain self-tests that are more robust to noise. Indeed, given the families of Bell expressions able to self-test the partially entangled state of two qubits that we discovered with the SOS method, it is natural to ask which of these is most robust to noise. In fact, it would be interesting to answer this question both for a fixed set of measurement settings and for arbitrary measurements.

Finally, the constraints imposed by the SOS method apply to both the state and measurements parameters. Therefore, the method can be used to construct inequalities tailored to target measurements as well, such as families of Bell expressions for fixed settings and varying states [75]. It would be interesting to further investigate the relevance of the SOS method to self-testing of measurements.

## Geometry of the quantum set of correlations

Understanding the set of quantum correlations is of both fundamental and practical importance. In this thesis, we provided an analytical description of the quantum set in one of its most popular scenario. Moreover, we proved that all extremal points in this scenario self-test a two qubit realization. To obtain these results, we have used a non-linear steering transformation of the correlations, which appears to capture an intrinsic property of quantum correlations. This technique offers a promising perspective for the study of quantum correlations in broader scenarios. One direct generalization would be to investigate whether the results obtained here can be extended to describe the set of qubit correlations for two parties, two settings and an arbitrary number of measurement settings following steps similar to [102].

We provided an analytical description of the boundary of the quantum set in the CHSH scenario through a non-linear function. It will be interesting to find out whether an analytical boundary of the set can also be expressed for the quantum set with additional parties, inputs or outputs. For instance, it has been proven that the boundary of the  $(2, 5, 3)$ -Bell scenario requires quantum systems of arbitrarily large dimension [103].

While this work offers a first analytical insight on the quantum set, much remains to be done to obtain a full geometrical understanding of this object. For instance, it remains an open question to determine the level at which the NPA hierarchy is tight in the CHSH scenario [57]. Our work could provide an important step towards this line. Another open question concerns an analytical description of the dual of the quantum set. This set is of foremost importance for many quantum information protocols, as it encodes the Tsirelson bounds of all Bell expressions. In chapter 4, we studied the quantum set  $\mathcal{Q}$  from a dual perspective. In particular, we derived constructively all the Bell expressions that the Tsirelson point  $\vec{P}_T$  maximizes. This provides fresh insight on the geometry of the quantum set. In particular, we show analytically that  $\vec{P}_T$  is an extremal point of  $\mathcal{Q}$  of dual dimension 2 that lies at the top of a pyramid. This geometrical picture goes against many representations that were given of this point in other projections. The new Bell expressions found with the SOS method allowed us to demonstrate that a family of points corresponding to the partially entangled states are also angulous points of the quantum set. This implies that their dual dimension is at least one, and we proved in chapter 4 it is actually upper bounded by two. It would be interesting to find out whether it is a generic property of exposed extremal quantum statistics to have a non-zero dual dimension.

Our work also identifies 8 exposed extremal points of  $\mathcal{Q}^*$ , all of dual dimension 2 as well, thus fully describing a face of  $\mathcal{Q}^*$  of dimension 2. To our knowledge, this is the first time that nonlocal extremal points of the quantum dual are highlighted. Our work also answers an important question about the relation between  $\mathcal{Q}$  and  $\mathcal{Q}^*$  first raised in [20]. In this work, a linear map was introduced to prove that  $\mathcal{L}^* \cong \mathcal{NS}$ . Since this map sends the extremal point  $\vec{P}_T$  onto the non-extremal inequality  $\beta_{\text{CHSH}}/2\sqrt{2}$ , and linear isomorphisms preserve extremality, this shows that this application cannot be used to map  $\mathcal{Q}$  to  $\mathcal{Q}^*$ . This suggests that the quantum set  $\mathcal{Q}$  might not be self-dual after all, and that  $\mathcal{Q}^*$  may have a very different geometry.



## Outlooks

As shown in this thesis, the use of mathematical tools, such as duality, combined with innovative ideas rooted in quantum mechanics, such as steering, can lead to great progress in the description of what quantum theory can achieve in Bell scenarios. Yet, in the end, the main conclusion may be that the study of the quantum correlations in this framework still has a long way to go. Even though most of our contributions focus on the CHSH scenario, we anticipate that the results presented in this thesis will help to improve our understanding of the quantum set beyond this scenario.

Our analytical description of the set still has a lot of potential applications. Starting back over 30 years ago, a single Bell inequality, the CHSH one, from which we gave the name of the corresponding scenario, has been fiercely studied for numerous applications, from certification of quantum systems to randomness generation. However, it is now known that the CHSH score, a single linear function of the correlations, may not always be the best suited for all these tasks [56]. The certification of partially entangled state as well as different measurement settings requires new Bell expressions [65]. Also, one cannot have two bits of shared randomness with a maximal CHSH violation and only two measurements per party, while tailored Bell expressions can certify up to two bits with CHSH values arbitrary close to 2 [87]. More recent works have emphasized that all these applications benefit from the use of the value of multiple Bell expressions at the same time [45] or even from the knowledge of the full probability distribution [104, 105]. Our work provides for the first time a way to consider analytically every possible realization that may lead to a given vector of correlations. As such, our work does not only have fundamental implications on quantum theory, but also opens the possibilities for new ways of analyzing key quantities underlying quantum information protocols. These call for further investigation.

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