Calculation and Application of New Quantum Bounds

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We review, correct, and develop an algorithm which determines arbitrary Quantum Bounds, based on the seminal work of Tsirelson [Lett. Math. Phys. **4**, 93 (1980)]. The vast potential of this algorithm is demonstrated by deriving both new number-valued Quantum Bounds, as well as identifying a new class of function-valued Quantum Bounds. Those results facilitate an 8-dimensional Volume Analysis of Quantum Mechanics which extends the work of Cabello [PRA **72** (2005)]. Finally we contrast the Volume defined be these bounds to that defined by the criteria of Navascués et al [NJP **10** (2008)], proving the function-valued Quantum Bounds to be more complete.

The EPR-Bell scenario [1–3] is now recognized as the fundamental kernel of nonlocal quantum behavior. As an abstract experiment it consists of two *spatially separated* experimenters (Alice and Bob), each having access to two apparatuses (A_0/A_1 and B_0/B_1) capable of only ±1 measurement outcomes. We may implement the scenario via spin measurements on a pair of entangled particles, where the A_i and B_i measure against some orientation angles θ_{A_i} and θ_{B_i} respectively. To ensure that Alice and Bob are not causally connected we demand that in every trial Alice and Bob choose between their available apparatuses at random at some preordained simultaneous instant. Each party builds up a pair of statistical estimates for the variables $P(A_0 = 1)$ and $P(A_1 = 1)$ or $P(B_0 = 1)$ and $P(B_1 = 1)$. By comparing individual trial results they determine the four additional statistical probabilities $P(A_i = B_j)$ for $i, j = 0, 1$. Here we follow the conventional notation of *expectation values* such that $\langle A_i\rangle \equiv P(A_i = 1) - P(A_i = -1)$ and $\langle A_i = B_j\rangle \equiv \langle A_i \cdot B_j\rangle$.

This paper provides a new and more complete answer to the question of *"What are the possible values for these eight expectation variables?"*. That question is the focal point of monumental historical controversy, and is a question which lacks a complete answer in the framework of Quantum Mechanics even today. We briefly review the question's history, including a partial answer from Quantum Mechanics, to provide the context for the achievements of this work.

The lack of causal connection between Alice and Bob during the trial is equivalent to stating that their individual local measurement values cannot reveal any information regarding the other's choice of apparatus. In 1935 Einstein et al [1] assumed that this communication restriction was equivalent to the a *Local Hidden Variable Model* (LHVM), which claims that all measurements merely reveal pre-established values. There are $4^2 = 16$ possible pre-determined-value 'sets' addressing the four *marginal* measurements $\langle A_0\rangle = \pm1, \langle A_1\rangle = \pm1, \langle B_0\rangle = \pm1, \langle B_1\rangle = \pm1$. Each such set necessarily includes the associated values for the four *joint* measurements $\langle A_i \cdot B_j\rangle$. By examining linear combinations of those 16 sets we find that *according to LHVM*

$$\langle A_0 \cdot B_0\rangle + \langle A_0 \cdot B_1\rangle + \langle A_1 \cdot B_0\rangle - \langle A_1 \cdot B_1\rangle \le 2\,. \quad (1)$$

This is an example of a "Bell"-type inequality [2, 3].

Bell first identified this formalism in 1964 [2] but then further recognized that the lack of causal connection, defined by the *No-Signaling* criteria (NOSIG), encompassed more possibilities than any LHVM theory could account for. He saw that the above inequality could still be violated without any signaling between the two parties. An extreme example [4, 5] of nonlocal but not signaling experimental behavior is as follows: So long as $\langle A_0\rangle = \langle A_1\rangle = \langle B_0\rangle = \langle B_1\rangle = 0$ one could still imagine $1 = \langle A_0 \cdot B_0\rangle = \langle A_0 \cdot B_1\rangle = \langle A_1 \cdot B_0\rangle = -\langle A_1 \cdot B_1\rangle$. In such a hypothetical experimental behavior all the local measurements would be utterly random, but fully correlated in 3/4 of the apparatus pairings, and yet somehow fully anti-correlated in the other. Contrary to instinct, this form of nonlocal correlation does not afford Alice any insight into Bob's choice of measurement apparatus, and vice versa, and is thus consistent with relativistic physics. Thus it was shown that *according to NOSIG*

$$\langle A_0 \cdot B_0\rangle + \langle A_0 \cdot B_1\rangle + \langle A_1 \cdot B_0\rangle - \langle A_1 \cdot B_1\rangle \le 4\,. \quad (2)$$

No such experimental behavior has ever been observed, and various theories which extend beyond NOSIG [6–8] claim it to be impossible.

Quantum Mechanics (QM) is an inextricably nonlocal theory. In 1980 Tsirelson generalized the Bell inequalities and found that *according to QM*

$$\langle A_0 \cdot B_0\rangle + \langle A_0 \cdot B_1\rangle + \langle A_1 \cdot B_0\rangle - \langle A_1 \cdot B_1\rangle \le 2\sqrt{2} \quad (3)$$

a result known as "Tsirelson's Bound". One can saturate the quantum inequality by considering the entangled qubit $(|00\rangle - |11\rangle)/\sqrt{2}$ with spin measurements $\theta_{A_0} = 0°, \theta_{A_1} = 90°, \theta_{B_1} = -45°, \theta_{B_1} = +45°$. This satisfies $\langle A_0\rangle = \langle A_1\rangle = \langle B_0\rangle = \langle B_1\rangle = 0$ but only achieves $\cos(45°) = \sqrt{2}/2 = \langle A_0 \cdot B_0\rangle = \langle A_0 \cdot B_1\rangle = \langle A_1 \cdot B_0\rangle =$

$-\langle A_1 \cdot B_1 \rangle$, thus achieving the bound.

While Bell's inequalities *completely* characterize the distinctions between LHVM and NOSIG, the same is not true for the Quantum generalizations of those inequalities. Although we know that causal separation is enforced in Quantum Mechanics by the commutation of measurement operators [9, 10], translating that abstract principle into an equivalent and finite set of inequalities has not yet been possible. Note that Bell's inequalities are statements pertaining exclusively to the four *joint* expectation variables, those pertaining to correlations, which we shall call 4-Space. Whereas QM as a theoretical framework, on the other hand, refers inextricable and non-trivially to the other four *marginal* expectations as well; QM demands description in the entire 8-Space.

Many works [11–16] address descriptions of QM in the 4-Space of correlations, in which *marginal* expectation values are held fixed to zero. A set of *fully complete* conditions in 4-Space are known as the "TLM" criteria after Tsirelson [13], Landau [14], and Masanes [15]) who each derived an equivalent form of them independently. In contrast the field of characterizing QM in 8-Space has been less developed. Tsirelson shared a theorem on the matter in 1980 [17] followed by the hierarchy of semi-definite-programming tests of Navascués, Pironio, and Acín (NPA) in 2007 [18, 19], which converge in their infinite limit to a complete characterization of QM. Application of NPA algorithm yielded the NPA criteria, the first and only known inequalities in 8-Space. Those criteria have been used since as a 'gold standard', such as in Ref. [20], but one should not mistake them for complete.

To obtain the more complete characterization of Quantum Mechanics given in this paper we returned to Theorem 2 of Tsirelson's 1980 work [17], which provides equivalent expressions for the upper limit on any linear combination of expectation values in 8-Space. Tsirelson's theorem was published without proof. In requisitioning the theorem for algorithmic development we identified a critical mathematical error which had been heretofore unnoticed. In this paper we construct the algorithm from first principles thus providing both proof and correction to Tsirelson's theorem. The specific repaired expressions appear in equation (9) here. Beyond pedagogically sharing the algorithm we report that initial applications of it have already tightened the characterization of QM in 8-Space. We present here new number-valued Quantum Bounds as well as a new class of function-valued Quantum Bounds.

More than three quarters of a century ago Einstein *et al.* asked *"Can Quantum-Mechanical Description of Physical Reality be Considered Complete?"* [1]. Their question is still being answered, and herein we provide the most complete descriptions of Physical Reality to date.

Tsirelson's theorem [17] provides equivalent formulations for the upper limit on any linear combination of expectation values in 8-Space. As an algorithm it is a method for answering the following general question: Given an arbitrary *8-space measure* $\langle Z \rangle$, defined by real number parameters c_i, such that

$$Z \equiv \; c_1 A_0 + c_2 A_1 + c_3 B_0 + c_4 B_1 + c_5\, A_0 \cdot B_0 + c_6\, A_1 \cdot B_0 + c_7\, A_0 \cdot B_1 + c_8\, A_1 \cdot B_1 \tag{4}$$

what is the upper limit on $\langle Z \rangle$; what is $\langle Z \rangle_{\text{Max}} =$?

For instance, choosing $1 = c_5 = c_6 = c_7 = -c_8$ with all the other $c_i = 0$ yields the example discussed in the introduction. For such a parameter set our algorithm should be able to reproduce the Quantum Bound given in equation (3). We note here that determining upper bounds for such linear combinations of expectation values is a relatively straightforward problem in both LHVM and NOSIG theories, as there exist well known inequalities [5, 21–24] which perfectly define those theories in 8-Space. It is computationally straightforwardly to maximize the linear function of expectation values subject to appropriate inequalities. No such perfectly-defining inequalities exist yet in Quantum Mechanics, hence the need for a unique algorithm, which we present here.

The key to the algorithm is the reduction of the abstract scenario of four apparatuses into four quantum measurement operators. The spatial separation requirement is enforced, as always, in the condition that the operators A_i and B_i commute with each other. In practice we go ahead and put the operators in separate Hilbert spaces, although for non-finite measurement values this may be too restrictive, see Refs. [9, 10]. The ± 1 possible measurements are embedded in the operators' eigenvalues, e.g. spin projectors to the x and y spin axes. Tsirelson proved that a 2-dimensional Hilbert space for each party was sufficient to emulate any general correlation behavior. Without loss of generality we can impose a reflection symmetry, so that

$$\begin{aligned} A_0 &\equiv (\cos(\theta)\sigma_x + \sin(\theta)\sigma_y) \otimes \mathbb{1}, \\ A_1 &\equiv (\cos(-\theta)\sigma_x + \sin(-\theta)\sigma_y) \otimes \mathbb{1}. \end{aligned} \tag{5}$$

In terms of unitary complex variables we write

$$\begin{aligned} A_0 &= \begin{pmatrix} 0 & u \\ \bar{u} & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad A_1 = \overline{A_0} \\ B_0 &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & v \\ \bar{v} & 0 \end{pmatrix} \quad B_1 = \overline{B_0}\,. \end{aligned} \tag{6}$$

Now, the 8-Space measure $\langle Z \rangle$ of Eq. (4) can be maximized over u and v.

The Quantum Bound is the largest possible measurement value of Z, which we can find by determining the largest root of the (4-dim) secular equation of Z and seeking out its global maximum variation over both u and v. With the characteristic polynomial Z written in terms of the variable m we have the quantum bound given by

$$\begin{aligned}\langle Z\rangle_{\text{Max}} = \sup(m) \quad \text{where} \quad \exists\, |u| = |v| = 1 \\ \text{such that} \quad m^4 + \mu_2 m^2 + \mu_3 m + \mu_4 \;=\; 0\end{aligned} \tag{7}$$

where here

$$\begin{aligned}\mu_2 &= -\left(|e|^2 + |f|^2\right) - 2\left(|g|^2 + |h|^2\right) , \\ \mu_3 &= 4\,\text{Re}\big[f h \bar{g} + e \bar{h} \bar{g}\big] , \\ \mu_4 &= |e|^2 |f|^2 + \left(|g|^2 - |h|^2\right)^2 - 2\,\text{Re}\big[f \bar{e} h^2 + e f \bar{g}^2\big] ,\end{aligned} \tag{8}$$

and where

$$\begin{aligned}e &= u v c_5 + v \bar{u} c_6 + u \bar{v} c_7 + \bar{u} \bar{v} c_8 , \\ f &= u \bar{v} c_5 + \bar{u} \bar{v} c_6 + u v c_7 + v \bar{u} c_8 , \\ g &= u c_1 + \bar{u} c_2 , \\ h &= v c_3 + \bar{v} c_4 .\end{aligned} \tag{9}$$

This, however, requires the analytically-intractable steps of identifying the largest solution to a quartic equation as well as maximizing over two variables. We bypass both obstacles through the use of *for all* statements, shifting the variation from both u and v to only m. Our characteristic polynomial has a definite positive leading coefficient (i.e. 1), and thus the quartic's largest solution is that for which all the derivatives are non-negative. As such, the quantum bound is given by the alternative formulation

$$\begin{aligned}\langle Z\rangle_{\text{Max}} = \sup(m) \quad \text{such that} \quad \forall\, |u| = |v| = 1 : \\ m^4 + \mu_2 m^2 + \mu_3 m + \mu_4 \;&\geq\; 0 \\ \text{and} \qquad 4m^3 + 2\mu_2 m + \mu_3 \;&\geq\; 0 \\ \text{and} \qquad 6m^2 + \mu_2 \;&\geq\; 0 \\ \text{and} \qquad m \;&\geq\; 0\end{aligned} \tag{10}$$

which is suitable for analytic analysis, in contrast to the formulation in (7).

Our ambition is to identify the Quantum Bound for all unitary (± 1) or zero values for the eight linear weights. These discrete (and finite) values are selected in effort to seek out *new* linear restrictions imposed by Quantum Mechanics. A naive approach would be the computation and collection of all $3^8 = 6561$ bounds, which, however, can be reduced to only ten fundamental non-trivial linear weightings by the use of symmetries. We list in Table I those three which are non-trivial, *i.e.*, those where the QM and NOSIG bounds do not coincide. The first of these is the well-known Tsirelson's Bound, but the latter two are new to the 8-Space analysis.

Note that for the last of the number-valued bounds listed here demonstrates zero non-locality beyond the *LHV* models. This would allow for an "inverse Hardy"-type [25, 26] all-or-nothing test of Quantum Mechanics, in that the presence of any non-locality would not vindicate Quantum Mechanics, but rather contradict it for the parameter region in question.

The algorithm's most powerful feature is not in yielding number-valued Quantum Bounds; other numerical algorithms (see the supplementary material) can do so more efficiently. The more significant reward is that, when paired with the symbolic algebra prowess of Mathematica™, our algorithm unleashes a new class of *function-valued* Quantum Bounds. Three such function-valued Quantum Bounds are presented in Table I as well.

An important quantitative technique called *Volume Analysis* has been introduced in[16] which ranks the number of points in a probability space allowed in a given model. A "probability space" refers to some set of expectation variables under consideration, such as 4-Space and 8-Space. A "point" corresponds to a set of values for those expectation variables. A "model." such as LHVM, NOSIG, and QM, is comprised of a set of criteria (inequalities) that define and restrict the allowed expectation values. The relative volume between two models corresponds to the probability that a point allowed in the larger-volume model would also be contained in the smaller-volume model.[27] Volume Analysis has heretofore only been attempted in 4-Space, since comprehensive bounds for the 8-space did not exist. In this paper we resolved that obstacle by generating the function-valued Quantum Bounds to be used as an approximation for the QM model.

We can estimate the completeness of function-valued Quantum Bounds in general by calibrating them against known results. For example we expect that repeating the 4-Space Volume Analysis of Ref. [16] using the first of the function-valued Quantum Bounds in Table I should yield an estimate of the Quantum Volume much closer to to the *true* value (determined using the TLM criteria [13–15]) than an estimate determined using only the number-valued Tsirelson's Bound. Indeed we find the function-valued bound estimate of the 4-Space volume to be $\approx 0.951 \times 2^4$, a significant tightening compared to the volume of $\approx 0.961 \times 2^4$ determined from the number-valued Tsirelson's Bound alone. The *true* Quantum Volume in 4-Space is $\approx 0.925 \times 2^4$ [16].

To construct a model of Quantum Mechanics in 8-Space we combined our three function-valued Quantum Bounds of Table I with the TLM criteria [13–15] and general No-Signaling criteria. We then used high-precision Monte Carlo numerical integration over all eight expectation variables. The QM volume presented in Table II is very precise for the model as composed, but due to the incomplete nature of the model, is necessarily an overestimate of the *true* Quantum Volume in 8-Space. The LHVM and NOSIG volumes in Table II are exact, calculated through analytic integration.

Finally we note that the three function-valued Quantum Bounds in Table I compose a tighter restriction set to QM than the present standard – the NPA criteria [18, 19]. This is proven by contrasting the QM volume (in Table

TABLE I. Bounds (Number-Valued and Function-Valued): The first is Tsirelson's Bound and its function-valued generalization; the last is a set in which $\mathrm{QM}_{\mathrm{Max}}$ has zero non-locality, in that $\mathrm{QM}_{\mathrm{Max}} \not> \mathrm{LHVM}_{\mathrm{Max}}$.

c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	$\mathrm{LHVM}_{\mathrm{Max}}$	$\mathrm{QM}_{\mathrm{Max}}$	$\mathrm{NOSIG}_{\mathrm{Max}}$
0	0	0	0	1	1	1	-1	2	$2\sqrt{2}$	4
0	0	0	0	1	1	1	x	$\lvert x+1\rvert+2$	$\begin{cases} x+3 & \text{for } x \geq -\frac{1}{3} \\ \sqrt{\frac{x^3-3x^2+3x-1}{x}} & \text{for } x \leq -\frac{1}{3} \end{cases}$	$\lvert x\rvert+3$
1	0	0	0	1	1	1	-1	3	$\sqrt{10}$	4
x	0	0	0	1	1	1	-1	$\lvert x\rvert+2$	$\begin{cases} \lvert x\rvert+2 & \text{for } \lvert x\rvert \geq 2 \\ \sqrt{2x^2+8} & \text{for } \lvert x\rvert \leq 2 \end{cases}$	$\begin{cases} \lvert x\rvert+2 & \text{for } \lvert x\rvert \geq 2 \\ 4 & \text{for } \lvert x\rvert \leq 2 \end{cases}$
1	1	-1	0	1	1	1	-1	3	3	4
x	x	-x	0	1	1	1	-1	$\begin{cases} 3\lvert x\rvert-2 & \text{for } \lvert x\rvert \geq 2 \\ \lvert x\rvert+2 & \text{for } \lvert x\rvert \leq 2 \end{cases}$	$\begin{cases} 3\lvert x\rvert-2 & \text{for } \lvert x\rvert \geq 2 \\ \lvert x\rvert+2 & \text{for } 1 \leq \lvert x\rvert \leq 2 \\ \frac{x^2}{x^2-1}+\sqrt{\frac{3x^4-10x^2+8}{(x^2-1)^2}} & \text{for } \lvert x\rvert \leq 1 \end{cases}$	$\begin{cases} 3\lvert x\rvert-2 & \text{for } \lvert x\rvert \geq 2 \\ 4 & \text{for } \lvert x\rvert \leq 2 \end{cases}$

II) to the volume of a model defined by the NPA criteria. The NPA criteria states that, for all i and j,

$$\begin{aligned} &|\mathfrak{f}(A_0,B_0)+\mathfrak{f}(A_0,B_1)+\mathfrak{f}(A_1,B_0)+\mathfrak{f}(A_1,B_1) \\ &\quad -2\mathfrak{f}(A_i,B_j)| \leq \pi \text{ , where} \\ &\mathfrak{f}(A_i,B_j)=\sin^{-1}\left(\frac{\langle A_0B_0\rangle-\langle A_0\rangle\langle B_0\rangle}{\sqrt{(1-\langle A_0\rangle^2)(1-\langle B_0\rangle^2)}}\right). \end{aligned} \tag{11}$$

The volume found via these NPA criteria is $\mathrm{NPA}_{\mathrm{Vol}} \approx 1085.8 \times \frac{2^8}{8!}$, which, compared to NOSIG, excludes only a bit more than half as much volume than our function-valued Quantum Bounds.

To conclude, we have rederived, repaired, and repurposed Tsirelson's theorem [17] as an algorithm to obtain arbitrary Quantum Bounds, number- and function-valued. With those we found that the full eight dimensional joint probability space of the EPR-Bell scenario is at least 0.3% smaller in QM than would be allowed by No-Signaling.

The algorithm is presently limited exclusively to bipartite dichotomic binary experiments. While this is the most studied scenario we still desire a more scalable method. Multiple choices per party [12, 28] and multipartite scenarios [29–31] are expected to aid in defining limits of quantum eavesdroppers [32], and perhaps widening security parameters in the industry-standard six-state QKD protocol [33]. Partial progress has been made [12, 28].

TABLE II. Results of Volume Analysis. The entire probability space, within which No-Signaling theories are contained, has total volume $2^8 = 256$.

$\mathrm{LHVM}_{\mathrm{Vol}}$	$\mathrm{QM}_{\mathrm{Vol}}$	$\mathrm{NOSIG}_{\mathrm{Vol}}$
$= 1024 \times \frac{2^8}{8!}$	$\lesssim 1084.3 \times \frac{2^8}{8!}$	$= 1088 \times \frac{2^8}{8!}$

Aside from generalizations extending the EPR-Bell scenario there remains work to be done in the core characterization itself. The algorithm we share here is only one tool to approach a complete characterization, the convergent hierarchy of Navascués et al [19] is another. We eagerly anticipate the discover of necessary and sufficient nonlinear inequalities which will completely describe Quantum Mechanics in 8-Space just as the TLM criteria [13–15] do so in 4-Space.

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