Analytic and nearly optimal self-testing bounds for the Clauser-Horne-Shimony-Holt and Mermin inequalities (Supplemental Material)

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I. SUFFICIENCY OF CONSIDERING QUBIT OBSERVABLES

We want to argue that if the operator inequality (6) holds for qubit observables for all angles then it holds for all binary observables. For simplicity we sketch out the argument for the bipartite scenario but the multipartite generalisation is straightforward.

First note that we can without loss of generality assume that the measurements are projective (if they were not Alice and Bob would append local ancillas to make them projective). To avoid dealing with a direct sum of blocks of different size, for every trivial 1×1 block in the Jordan decomposition we add an extra dimension to the local Hilbert space. This simply corresponds to embedding the state in a larger Hilbert space (the state is not supported on these extra dimensions) but we can use these extra dimensions to turn every trivial block into some non-trivial block (the choice of the angle is irrelevant but for definiteness we can choose $a = b = 0$). Applying the same procedure on both sides ensures that we can write the operator K as

$$K = \sum_{xy} |x\rangle\langle x|_X \otimes |y\rangle\langle y|_Y \otimes K(a_x, b_y),$$

where X and Y are classical registers storing the block information of Alice and Bob respectively, a_x, b_y are the angles and $K(a_x, b_y)$ is a 4×4 operator corresponding to qubit observables. Similarly the Bell operator W can be written as

$$W = \sum_{xy} |x\rangle\langle x|_X \otimes |y\rangle\langle y|_Y \otimes W(a_x, b_y).$$

If the operator inequality

$$K(a, b) \geq sW(a, b) + \mu\mathbb{1}$$

holds for qubit observables for all angles $a, b \in [0, \pi/2]$, it immediately implies that

$$K \geq sW + \mu\mathbb{1}$$

holds for all observables.

II. OPERATOR INEQUALITIES FOR QUBIT OBSERVABLES

Propositions 1 and 2 constitute the main technical contributions of this work. The proofs rely exclusively on elementary linear algebra and analysis but the actual calculations are rather lengthy.

Let us start by outlining the general proof technique. We aim to show that for some specific values of s and μ the operator $T := K - sW - \mu\mathbb{1}$ is positive semidefinite for all angles between the local observables. In the first step we show that T admits a generic block-diagonalisation into two-dimensional blocks (generic in the sense that these subspaces do not depend on the angles). More concretely we propose a partition of the identity into two-dimensional projectors $\sum_x P_x = \mathbb{1}$ which commute with T ($[T, P_x] = 0$) for all x and for all angles. Therefore

$$T = \sum_x P_x T P_x$$

and it suffices to prove positivity of each block $M_x := P_x T P_x$. Since the rank of M_x is at most 2 we have

$$M_x \geq 0 \quad \iff \quad \operatorname{tr} M_x \geq 0 \ \wedge \ (\operatorname{tr} M_x)^2 - \operatorname{tr} M_x^2 \geq 0.$$

A. Proof of Proposition 1

The maximally entangled state Φ_{AB} is

$$\Phi_{AB} = \frac{1}{4}\Big(\mathbb{1}\otimes\mathbb{1} + \sigma_y\otimes\sigma_y + \frac{1}{\sqrt{2}}\big[\sigma_x\otimes\sigma_x + \sigma_z\otimes\sigma_x + \sigma_x\otimes\sigma_z - \sigma_z\otimes\sigma_z\big]\Big),$$

the dephased operator is $K(a,b) = \big(\Lambda_A(a)\otimes\Lambda_B(b)\big)(\Phi_{AB})$ and the Bell operator is

$$W(a,b) = 2\big(\cos a\cos b\cdot\sigma_x\otimes\sigma_x + \sin a\cos b\cdot\sigma_z\otimes\sigma_x + \cos a\sin b\cdot\sigma_x\otimes\sigma_z - \sin a\sin b\cdot\sigma_z\otimes\sigma_z\big).$$

Our goal is to show that the operator $T(a,b) = K(a,b) - sW(a,b) - \mu\mathbb{1}$ is positive semidefinite for

$$s = \frac{4+5\sqrt{2}}{16} \quad\text{and}\quad \mu = -\frac{1+2\sqrt{2}}{4}$$

for all $a,b\in[0,\pi/2]$. It is easy to check that

$$T(a,b) = (H\otimes\sigma_x)T(\pi/2-a,b)(H\otimes\sigma_x),$$

which means that if we only care about the positivity of the operator it suffices to consider the range $a\in[0,\pi/4]$. By symmetry the same argument works for b so from now on we assume that $a,b\in[0,\pi/4]$. Then the dephasing occurs in the Hadamard basis and we have

$$K(a,b) = \frac{1}{4}\Big(\mathbb{1}\otimes\mathbb{1} + g(a)g(b)\sigma_y\otimes\sigma_y + \frac{1}{\sqrt{2}}\big[\sigma_x\otimes\sigma_x + g(a)\sigma_z\otimes\sigma_x + g(b)\sigma_x\otimes\sigma_z - g(a)g(b)\sigma_z\otimes\sigma_z\big]\Big).$$

Writing $T(a,b)$ out gives

$$\begin{aligned} T(a,b) =& \Big(\frac{1}{4}-\mu\Big)\mathbb{1}\otimes\mathbb{1} + \frac{1}{4}g(a)g(b)\sigma_y\otimes\sigma_y + \frac{1}{4\sqrt{2}}\Big(\big[1-8s\sqrt{2}\cos a\cos b\big]\sigma_x\otimes\sigma_x + \big[g(a)-8s\sqrt{2}\sin a\cos b\big]\sigma_z\otimes\sigma_x \\ &+ \big[g(b)-8s\sqrt{2}\cos a\sin b\big]\sigma_x\otimes\sigma_z - \big[g(a)g(b)-8s\sqrt{2}\sin a\sin b\big]\sigma_z\otimes\sigma_z\Big). \end{aligned}$$

Noticing that $[T(a,b),\sigma_y\otimes\sigma_y]=0$ for all $a,b\in[0,\pi/2]$ leads us to consider projectors

$$P_x := \frac{1}{2}\big(\mathbb{1}\otimes\mathbb{1} + (-1)^x\sigma_y\otimes\sigma_y\big)$$

for $x\in\{0,1\}$. Then

$$\operatorname{tr} M_x = \operatorname{tr}\big(P_x T(a,b)\big) = \frac{1}{2} - 2\mu + (-1)^x\frac{g(a)g(b)}{2}$$

and clearly $\operatorname{tr} M_x \geq 0$ (because $\mu\leq 0$ and $g(a),g(b)\in[0,1]$). Computing $\operatorname{tr} M_x^2$ is slightly more involved but ultimately leads to

$$\begin{aligned} \operatorname{tr} M_x^2 = \operatorname{tr}\big(P_x[T(a,b)]^2\big) = 2\bigg[&\Big(\frac{1}{4}-\mu\Big)^2 + \frac{1+g(a)^2+g(b)^2+3\big[g(a)g(b)\big]^2}{32} + 4s^2 - \frac{s}{\sqrt{2}}(\cos a + g(a)\sin a)(\cos b + g(b)\sin b)\bigg] \\ &+ \frac{(-1)^x}{2}\Big[(1-2\mu)g(a)g(b) - 2s\sqrt{2}\big[g(a)\cos a + \sin a\big]\big[g(b)\cos b + \sin b\big] + 16s^2\sin 2a\sin 2b\Big]. \end{aligned}$$

Our goal is to show the positivity of $\lambda_x(a,b) := (\operatorname{tr} M_x)^2 - \operatorname{tr} M_x^2$ for $x\in\{0,1\}$ and $a,b\in[0,\pi/4]$. Writing the entire expression out gives

$$\begin{aligned} \lambda_x(a,b) = 2\Big(\frac{1}{4}-\mu\Big)^2 &+ \frac{-1-g(a)^2-g(b)^2+\big[g(a)g(b)\big]^2}{16} - 8s^2 + s\sqrt{2}(\cos a + g(a)\sin a)(\cos b + g(b)\sin b) \\ &+ (-1)^x\Big[-\mu g(a)g(b) + s\sqrt{2}\big[g(a)\cos a + \sin a\big]\big[g(b)\cos b + \sin b\big] - 8s^2\sin 2a\sin 2b\Big]. \end{aligned}$$

It is convenient to introduce new coordinates: $u = (a+b)/2$ and $t = \cos[(a-b)/2]$. The domain $(a,b)\in[0,\pi/4]$ maps onto $u\in[0,\pi/4]$ and

$$t \in \big[\cos\big(\min\{u,\pi/4-u\}\big), 1\big]$$

but for simplicity we extend it to $t\in[\zeta,1]$ for $\zeta=\cos(\pi/8)$.

- For $x=0$ we have

$$\lambda_0(u,t) = \frac{15+12\sqrt{2}}{2}t^4 - 2(10+7\sqrt{2})(\sin u+\cos u)t^3 + \left(\frac{27+17\sqrt{2}}{2} + \frac{27+19\sqrt{2}}{2}\sin 2u\right)t^2$$
$$- \left((3+2\sqrt{2})\sin u - \frac{2+\sqrt{2}}{2}\cos u - \frac{8+5\sqrt{2}}{2}(\sin u-\cos u)(\sin u)^2\right)t$$
$$- \frac{4+3\sqrt{2}}{2}\sin 2u + \frac{2+\sqrt{2}}{4}\cos 4u - \frac{10+5\sqrt{2}}{4}.$$

To prove $\lambda_0(u,t)\geq 0$ for $u\in[0,\pi/4]$ and $t\in[\zeta,1]$ we lowerbound it by a quadratic function. First we check that $\lambda_0(u,\zeta)\geq\lambda_0(u,1)\geq 0$ (for all $u\in[0,\pi/4]$), which implies that the quadratic function

$$q(u,t) := \big[\lambda_0(u,\zeta)-\lambda_0,(u,1)\big]\left(\frac{1-t}{1-\zeta}\right)^2 + \lambda_0(u,1)$$

is non-negative. The final step is to verify that the difference $h(u,t):=\lambda_0(u,t)-q(u,t)$ is non-negative $h(u,t)\geq 0$, which follows directly from vanishing on the boundary ($h(u,\zeta)=h(u,1)=0$) and concavity (check that $\partial^2 h/\partial t^2\leq 0$).

- For $x=1$ we have

$$\lambda_1(u,t) = \frac{25+16\sqrt{2}}{2}t^4 - \frac{1}{2}\big[(8+5\sqrt{2})\sin u + (26+19\sqrt{2})\cos u\big]t^3$$
$$+ \frac{1}{4}\big[-(38+24\sqrt{2}) + (31+22\sqrt{2})\sin 2u - (23+16\sqrt{2})\cos 2u\big]t^2$$
$$+ \frac{1}{2}\big[-(2+2\sqrt{2})\sin u + (33+24\sqrt{2})\cos u - (40+28\sqrt{2})(\sin u)^2\cos u - (6+4\sqrt{2})(\sin u)^3\big]t$$
$$- \frac{19+14\sqrt{2}}{8}\sin 2u + \frac{5+2\sqrt{2}}{8}\cos 2u - \frac{23+16\sqrt{2}}{16}\sin 4u - \frac{25+16\sqrt{2}}{16}\cos 4u + \frac{3+4\sqrt{2}}{16}.$$

It is easy to verify that $\lambda_1(u,t)$ is convex in t (check that $\partial^2\lambda_1/\partial t^2>0$) which means it can be lowerbounded by linear functions tangent to it. Checking these at $t=\zeta$ and $t=1$ suffices to prove positivity.

B. Proof of Proposition 2

The optimal state Υ_{ABC} is

$$\Upsilon_{ABC} = \frac{1}{8}\big(\mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1} + \sigma_y\otimes\sigma_y\otimes\mathbb{1} - \sigma_y\otimes\mathbb{1}\otimes\sigma_y - \mathbb{1}\otimes\sigma_y\otimes\sigma_y\big)$$
$$+ \frac{1}{8\sqrt{2}}\big(\sigma_x\otimes\sigma_x\otimes\sigma_x - \sigma_x\otimes\sigma_x\otimes\sigma_z + \sigma_x\otimes\sigma_z\otimes\sigma_x + \sigma_z\otimes\sigma_x\otimes\sigma_x$$
$$+ \sigma_x\otimes\sigma_z\otimes\sigma_z + \sigma_z\otimes\sigma_x\otimes\sigma_z - \sigma_z\otimes\sigma_z\otimes\sigma_x + \sigma_z\otimes\sigma_z\otimes\sigma_z\big),$$

the dephased operator is $K(a,b,c) = \big(\Lambda_A(a)\otimes\Lambda_B(b)\otimes\Lambda_C(c)\big)(\Upsilon_{ABC})$ and the Bell operator is

$$W = 2\big(\cos a\cos b\cos c\,\sigma_x\otimes\sigma_x\otimes\sigma_x - \cos a\cos b\sin c\,\sigma_x\otimes\sigma_x\otimes\sigma_z + \cos a\sin b\cos c\,\sigma_x\otimes\sigma_z\otimes\sigma_x$$
$$+ \sin a\cos b\cos c\,\sigma_z\otimes\sigma_x\otimes\sigma_x + \cos a\sin b\sin c\,\sigma_x\otimes\sigma_z\otimes\sigma_z + \sin a\cos b\sin c\,\sigma_z\otimes\sigma_x\otimes\sigma_z$$
$$- \sin a\sin b\cos c\,\sigma_z\otimes\sigma_z\otimes\sigma_x + \sin a\sin b\sin c\,\sigma_z\otimes\sigma_z\otimes\sigma_z\big).$$

Our goal is to show that the operator $T(a,b,c) = K(a,b,c) - sW(a,b,c) - \mu\mathbb{1}$ is positive semidefinite for

$$s = \frac{2+\sqrt{2}}{8} \quad \text{and} \quad \mu = -\frac{1}{\sqrt{2}}$$

for all $a,b,c\in[0,\pi/2]$. It is easy to check that

$$T(a,b,c) = (H\otimes\sigma_x\otimes\sigma_x)T(\pi/2-a,b,c)(H\otimes\sigma_x\otimes\sigma_x)$$
$$= (\sigma_x\otimes H\otimes\sigma_x)T(a,\pi/2-b,c)(\sigma_x\otimes H\otimes\sigma_x)$$
$$= (\sigma_x\otimes\sigma_x\otimes V)T(a,b,\pi/2-c)(\sigma_x\otimes\sigma_x\otimes V),$$

where $V = (\sigma_x - \sigma_z)/\sqrt{2}$. Therefore it suffices to consider $a, b, c \in [0, \pi/4]$. Then the dephasing occurs in the Hadamard basis and we have

$$\begin{aligned}K(a,b,c) &= \frac{1}{8}\big(\mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1} + g(a)g(b)\sigma_y\otimes\sigma_y\otimes\mathbb{1} - g(a)g(c)\sigma_y\otimes\mathbb{1}\otimes\sigma_y - g(b)g(c)\mathbb{1}\otimes\sigma_y\otimes\sigma_y\big)\\ &+ \frac{1}{8\sqrt{2}}\big(\sigma_x\otimes\sigma_x\otimes\sigma_x - g(c)\sigma_x\otimes\sigma_x\otimes\sigma_z + g(b)\sigma_x\otimes\sigma_z\otimes\sigma_x + g(a)\sigma_z\otimes\sigma_x\otimes\sigma_x\\ &+ g(b)g(c)\sigma_x\otimes\sigma_z\otimes\sigma_z + g(a)g(c)\sigma_z\otimes\sigma_x\otimes\sigma_z - g(a)g(b)\sigma_z\otimes\sigma_z\otimes\sigma_x + g(a)g(b)g(c)\sigma_z\otimes\sigma_z\otimes\sigma_z\big).\end{aligned}$$

Noticing that $[T(a,b,c), \mathbb{1}\otimes\sigma_y\otimes\sigma_y] = [T(a,b,c), \sigma_y\otimes\mathbb{1}\otimes\sigma_y] = [T(a,b,c), \sigma_y\otimes\sigma_y\otimes\mathbb{1}] = 0$ for all $a, b, c \in [0, \pi/2]$ leads us to consider projectors

$$P_{x_1x_2} = \frac{1}{4}\big(\mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1} + (-1)^{x_1}\sigma_y\otimes\sigma_y\otimes\mathbb{1} + (-1)^{x_2}\sigma_y\otimes\mathbb{1}\otimes\sigma_y + (-1)^{x_1+x_2}\mathbb{1}\otimes\sigma_y\otimes\sigma_y\big)$$

for $x_1, x_2 \in \{0, 1\}$. It is easy to check that

$$\operatorname{tr} M_{x_1,x_2} = \operatorname{tr}\big(P_{x_1,x_2}T(a,b,c)\big) = 2\left(\frac{1}{8} - \mu\right) + \frac{1}{4}\big[(-1)^{x_1}g(a)g(b) - (-1)^{x_2}g(a)g(c) - (-1)^{x_1+x_2}g(b)g(c)\big],$$

which is easily seen to be positive

$$\operatorname{tr} M_{x_1,x_2} \geq 2\left(\frac{1}{8} - \mu\right) - \frac{3}{4} \geq 0.$$

Computing $\operatorname{tr} M^2_{x_1,x_2}$ is a rather lengthy calculation so let us go directly to the final expression. Our goal is to show the positivity of $\lambda_{x_1,x_2}(a,b,c) := (\operatorname{tr} M_{x_1,x_2})^2 - \operatorname{tr} M^2_{x_1,x_2}$ for $x_1, x_2 \in \{0, 1\}$ and $a, b, c \in [0, \pi/4]$. Writing the entire expression out gives

$$\begin{aligned}\lambda_{x_1x_2}(a,b,c) &= 2\left(\frac{1}{8} - \mu\right)^2 - \frac{1}{32} + \frac{[1-g(a)^2][1-g(b)^2][1-g(c)^2]}{64}\\ &- 8s^2 + \frac{s}{\sqrt{2}}[\cos a + g(a)\sin a][\cos b + g(b)\sin b][\cos c + g(c)\sin c]\\ &+ (-1)^{x_1}\left[-\frac{\mu g(a)g(b)}{2} - 8s^2\sin 2a\sin 2b + \frac{s}{\sqrt{2}}[g(a)\cos a + \sin a][g(b)\cos b + \sin b][\cos c + g(c)\sin c]\right]\\ &+ (-1)^{x_2}\left[\frac{\mu g(a)g(c)}{2} + 8s^2\sin 2a\sin 2c - \frac{s}{\sqrt{2}}[g(a)\cos a + \sin a][\cos b + g(b)\sin b][g(c)\cos c + \sin c]\right]\\ &+ (-1)^{x_1+x_2}\left[\frac{\mu g(b)g(c)}{2} + 8s^2\sin 2b\sin 2c - \frac{s}{\sqrt{2}}[\cos a + g(a)\sin a][g(b)\cos b + \sin b][g(c)\cos c + \sin c]\right].\end{aligned}$$

First we observe that the cases $(x_1, x_2) \in \{(0,0), (1,0), (1,1)\}$ are equivalent in the sense that

$$\lambda_{00}(a,b,c) = \lambda_{10}(c,b,a) = \lambda_{11}(a,c,b).$$

Therefore it suffices to prove positivity of one of them (for all $a, b, c \in [0, \pi/4]$). The case of $x_1 = 0, x_2 = 1$ is qualitatively different and turns out to be strictly more restrictive then the other ones. To show this we first prove that

$$\Delta\lambda(a,b,c) := \lambda_{00}(a,b,c) - \lambda_{01}(a,b,c) \geq 0$$

for all $a, b, c \in [0, \pi/4]$. Computing the difference gives

$$\begin{aligned}\Delta\lambda(a,b,c) &= \mu[g(a) + g(b)]g(c) + 16s^2(\sin 2a + \sin 2b)\sin 2c\\ &- s\sqrt{2}[g(c)\cos c + \sin c]\Big([g(a) + g(b)]\cos(a-b) + [1 + g(a)g(b)]\sin(a+b)\Big).\end{aligned}$$

Since the case of $c = 0$ is trivial (all the terms vanish), we divide through by $\sin 2c$. It is easy to verify that

$$\begin{aligned}\frac{g(c)}{\sin 2c} &\leq \frac{1+\sqrt{2}}{2},\\ \frac{g(c)\cos c + \sin c}{\sin 2c} &\leq \frac{2+\sqrt{2}}{2}.\end{aligned}$$

Applying these inequalities and using the substitution of variables mentioned before ($u = (a+b)/2$ and $t = \cos[(a-b)/2]$) gives

$$\frac{\Delta\lambda(u,t)}{2s\sin 2c} \geq f(u,t) := -(6+4\sqrt{2})(\sin u + \cos u)t^3 + \big[6+4\sqrt{2} + (1-\sqrt{2})\sin 2u\big]t^2 + (\sin u + \cos u)\big[1 + (7+5\sqrt{2})\sin 2u\big]t$$
$$- \frac{9+5\sqrt{2}}{2}\sin 2u - \frac{7+5\sqrt{2}}{2}(\sin 2u)^2 - 1.$$

The final step is to check that $f(u,t)$ is concave in t (check that $\partial^2 f/\partial t^2 \leq 0$) and then verify that the function is non-negative on the boundaries ($f(u,\zeta) \geq 0$ and $f(u,1) \geq 0$).

The last step is to prove that $\lambda_{01}(a,b,c) \geq 0$. In this case we use the substitution

$$x = 1 - \sin(a + \pi/4),$$
$$y = 1 - \sin(b + \pi/4),$$
$$z = 1 - \sin(c + \pi/4),$$

which maps the domain $a,b,c \in [0,\pi/4]$ onto $x,y,z \in [0,\eta]$ for $\eta := 1 - 1/\sqrt{2}$. This allows us to write

$$\lambda_{01}(a,b,c,x,y,z) = P(x,y,z) + Q(a,b,c)$$

where

$$P(x,y,z) := (3+2\sqrt{2})(xy+xz+yz) - \frac{4+3\sqrt{2}}{2}(x^2y + x^2z + xy^2 + xz^2 + y^2z + yz^2)$$
$$+ \frac{4+3\sqrt{2}}{2}(x^2y^2 + x^2z^2 + y^2z^2) + \frac{69+48\sqrt{2}}{4}xyz(x+y+z)$$
$$- \frac{50+35\sqrt{2}}{8}xyz(xy+xz+yz) - \frac{128+87\sqrt{2}}{4}xyz - \frac{31+22\sqrt{2}}{8}x^2y^2z^2$$

and

$$Q(a,b,c) := \frac{2+\sqrt{2}}{8}[1-g(a)][1-g(b)][1-g(c)]\cos(a+\pi/4)\cos(b+\pi/4)\cos(c+\pi/4).$$

The second term is non-negative by inspection. To bound the polynomial term we first observe that

$$x^2y + x^2z + xy^2 + xz^2 + y^2z + yz^2 = (xy+xz+yz)(x+y+z) - 3xyz \leq 3\eta(xy+xz+yz) - 3xyz,$$

which implies

$$P(x,y,z) \geq \frac{3+\sqrt{2}}{2}(xy+xz+yz) + \frac{4+3\sqrt{2}}{2}(x^2y^2 + x^2z^2 + y^2z^2) + \frac{69+48\sqrt{2}}{4}xyz(x+y+z)$$
$$- \frac{50+35\sqrt{2}}{8}xyz(xy+xz+yz) - \frac{104+69\sqrt{2}}{4}xyz - \frac{31+22\sqrt{2}}{8}x^2y^2z^2.$$

In the final step we place a lower bound on this expression in terms of the geometric mean $r := \sqrt[3]{xyz}$. By the inequality of arithmetic and geometric means we have

$$x + y + z \geq 3r,$$
$$xy + yz + xz \geq 3r^2,$$
$$x^2y^2 + x^2z^2 + y^2z^2 \geq 3r^4.$$

Combining it with the trivial $xy + yz + xz \leq 3\eta^2$ implies $P(x,y,z) \geq P'(r)$ for

$$P'(r) := \frac{9+3\sqrt{2}}{2}r^2 - \frac{446+291\sqrt{2}}{16}r^3 + \frac{81\sqrt{2}}{2}r^4 - \frac{31+22\sqrt{2}}{8}r^6,$$

which is easily verified to be positive for $r \in [0,\eta]$.

III. COUNTEREXAMPLE TO THE UPPER BOUND

To show that the trivial upper bound is not achievable, we present a family of bipartite states that achieve the CHSH violation of $\beta \in (2, 2\sqrt{2})$ and argue that no extraction channels produce a singlet of fidelity reaching the upper bound (4). The following argument could probably be extended to give us an improved upper bound but this is beyond the scope of this work.

We consider a family of states in which each party holds two qubits. On each side the first qubit (labelled by X and Y respectively) is used as a classical register whereas the remaining qubits (labelled by A and B respectively) contain a quantum state. Consider the family of states

$$\rho_{XYAB} = \sum_{xy} p_{xy} |x\rangle\langle x|_X \otimes |y\rangle\langle y|_Y \otimes \tau_{AB}^{xy},$$

where $p_{11} = \nu$ and $p_{00} = p_{01} = p_{10} = (1-\nu)/3$ for $\nu \in (0,1)$ and the conditional states are

$$\begin{aligned}
\tau_{AB}^{00} &= \tau_{AB}^{01} = \tau_{AB}^{10} = \frac{1}{4}(\mathbb{1} \otimes \mathbb{1} + \sigma_x \otimes \sigma_x), \\
\tau_{AB}^{11} &= \frac{1}{4}\big(\mathbb{1} \otimes \mathbb{1} + \frac{1}{\sqrt{2}}[\sigma_x \otimes \sigma_x + \sigma_x \otimes \sigma_z + \sigma_z \otimes \sigma_x - \sigma_z \otimes \sigma_z] + \sigma_y \otimes \sigma_y\big).
\end{aligned}$$

The states $\tau_{AB}^{00}, \tau_{AB}^{01}, \tau_{AB}^{10}$ are perfectly (classically) correlated in the Hadamard basis, while τ_{AB}^{11} is a (pure) maximally entangled state. For simplicity we will assume that τ_{AB}^{11} is precisely the state that Alice and Bob are trying to extract. The observables of Alice and Bob are

$$\begin{aligned}
A_0 = B_0 &= |0\rangle\langle 0| \otimes \sigma_x + |1\rangle\langle 1| \otimes \sigma_x, \\
A_1 = B_1 &= |0\rangle\langle 0| \otimes \sigma_x + |1\rangle\langle 1| \otimes \sigma_z.
\end{aligned}$$

It is easy to verify that the CHSH value equals

$$\beta = 2 + (2\sqrt{2} - 2)\nu$$

and the value of the upper bound equals $(1+\nu)/2$. To reach it Alice and Bob would have to achieve the fidelity of 1 for $x = y = 1$ and of $\frac{1}{2}$ for the remaining states. We show that this is not possible.

Since the register X is classical, we can without loss of generality assume that the extraction channel applied by Alice is equivalent to a pair of qubit channels of the form $\{\Lambda^0_{A\to A'}, \Lambda^1_{A\to A'}\}$ corresponding to different values of x (and clearly an analogous argument holds for Bob). Therefore we have to optimise over two qubit channels for each party. In order to achieve the fidelity of 1 for $x = y = 1$ Alice and Bob must either do nothing or apply unitaries which leave the state τ_{AB}^{11} unchanged. Let us for now assume that they do nothing, i.e. that $\Lambda^1_{A\to A'}$ and $\Lambda^1_{B\to B'}$ are the identity channel. Once we know that $\Lambda^1_{B\to B'}$ is the identity channel, the only manner to achieve the optimal fidelity for $x = 0, y = 1$ is for Alice to apply a unital channel which satisfies

$$\Lambda^0_{A\to A'}(\sigma_x) = \frac{\sigma_x + \sigma_z}{\sqrt{2}}. \tag{1}$$

By symmetry considering the case of $x = 1, y = 0$ leads to the same conclusion for Bob. This determines all extraction channels and we can check that for $x = y = 0$ Alice and Bob end up with the state

$$\frac{1}{4}\big(\mathbb{1} \otimes \mathbb{1} + \frac{1}{2}[\sigma_x \otimes \sigma_x + \sigma_x \otimes \sigma_z + \sigma_z \otimes \sigma_x + \sigma_z \otimes \sigma_z]\big),$$

whose fidelity with τ_{AB}^{11} equals $\frac{1}{4} + \frac{1}{4\sqrt{2}}$ which is less than the desired $\frac{1}{2}$.

The case of Alice and Bob applying some non-trivial unitaries for $x = y = 1$ turns out to be similar: once $\Lambda^1_{A\to A'}$ and $\Lambda^1_{B\to B'}$ are fixed, we obtain constraints similar to Eq. (1) for $\Lambda^0_{A\to A'}$ and $\Lambda^0_{B\to B'}$. These constraints uniquely determine the state $(\Lambda^0_{A\to A'} \otimes \Lambda^0_{B\to B'})(\tau_{AB}^{00})$ and one can check that it always ends up being slightly "misaligned" with τ_{AB}^{11}.