3.4

(a)

$$
\begin{aligned}
|\langle\mathcal{B}\rangle| &= \big||\mathbf{b}-\mathbf{d}|\langle\boldsymbol{\sigma}\cdot\mathbf{a}\otimes\boldsymbol{\sigma}\cdot\mathbf{f}\rangle + |\mathbf{b}+\mathbf{d}|\langle\boldsymbol{\sigma}\cdot\mathbf{c}\otimes\boldsymbol{\sigma}\cdot\mathbf{g}\rangle\big| \\
&\le |\mathbf{b}-\mathbf{d}||\langle\boldsymbol{\sigma}\cdot\mathbf{a}\otimes\boldsymbol{\sigma}\cdot\mathbf{f}\rangle| + |\mathbf{b}+\mathbf{d}||\langle\boldsymbol{\sigma}\cdot\mathbf{c}\otimes\boldsymbol{\sigma}\cdot\mathbf{g}\rangle| \\
&\le |\mathbf{b}-\mathbf{d}| + |\mathbf{b}+\mathbf{d}| \\
&= \sqrt{2}\big(\sqrt{1-\mathbf{b}\cdot\mathbf{d}}+\sqrt{1+\mathbf{b}\cdot\mathbf{d}}\big) \\
&= \sqrt{2}\sqrt{\big(\sqrt{1-\mathbf{b}\cdot\mathbf{d}}+\sqrt{1+\mathbf{b}\cdot\mathbf{d}}\big)^2} \\
&= 2\sqrt{1+\sqrt{1-(\mathbf{b}\cdot\mathbf{d})^2}} \\
&\le 2\sqrt{2}
\end{aligned}
\tag{1}
$$

The mucking around here with the expressions involving $\mathbf{b}\cdot\mathbf{d}$ is just a way of getting the maximum without doing calculus. You could equally well do calculus on the the angle θ between $\mathbf{b}$ and $\mathbf{d}$, i.e., $\mathbf{b}\cdot\mathbf{d}=\cos\theta$.

(b) We need to look at the necessary and sufficient conditions for equality in the three inequalities in part (a). The condition for the first inequality is that the two correlation coefficients (expectation values) have the same sign. The second inequality comes from the fact that Pauli components have eigenvalues ±1 and thus that tensor products of Pauli components also have eigenvalues ±1. The maximum (minimum) expectation value of a Hermitian operator is the maximum (minimum) eigenvalue. The condition for the second inequality is thus that the expectation values have their maximum value $+1$ or their minimum value -1; by the condition on the first inequality, both correlation coefficients must be maximal or both must be minimal. This condition is achieved if and only if the joint quantum state $|\Psi\rangle$ of the two qubits is an eigenstate of the two tensor products with the same eigenvalue. Thus we conclude that the necessary and sufficient conditions for the first two inequalities are that

$$
\boldsymbol{\sigma}\cdot\mathbf{a}\otimes\boldsymbol{\sigma}\cdot\mathbf{f}|\Psi\rangle = \pm|\Psi\rangle \qquad \text{and} \qquad \boldsymbol{\sigma}\cdot\mathbf{c}\otimes\boldsymbol{\sigma}\cdot\mathbf{g}|\Psi\rangle = \pm|\Psi\rangle\ . \tag{2}
$$

The condition for the third inequality is that $\mathbf{b}\cdot\mathbf{d}=0$, i.e., that $\mathbf{b}$ and $\mathbf{d}$ are orthogonal. We could make the same argument exchanging the roles of the two qubits, P and Q, so we can also conclude that $\mathbf{a}$ and $\mathbf{c}$ are orthogonal. Thus we have that $\mathbf{a}$, $\mathbf{c}$, and $\mathbf{a}\times\mathbf{c}$ form a right-handed, orthogonal basis and likewise that $\mathbf{b}$, $\mathbf{d}$, and $\mathbf{b}\times\mathbf{d}$, or $\mathbf{f}=(\mathbf{b}-\mathbf{d})/\sqrt{2}$, $\mathbf{g}=(\mathbf{b}+\mathbf{d})/\sqrt{2}$, and $\mathbf{f}\times\mathbf{g}=\mathbf{b}\times\mathbf{d}$, form a right-handed, orthogonal basis. We could just declare at this point that we will rotate the Cartesian axes on each qubit so that these two right-handed, orthogonal sets are the local Cartesian axes. But we'll go at it in a way that finds the most general state given whatever Cartesian axes we started with.

To do this, we introduce a rotation R_P that rotates the standard basis $\{\mathbf{e}_x,\mathbf{e}_y,\mathbf{e}_z\}$ to the the right-handed basis $\{\mathbf{a},\mathbf{c},\mathbf{a}\times\mathbf{d}\}$ and another rotation R_Q that rotates the standard basis $\{\mathbf{e}_x,\mathbf{e}_y,\mathbf{e}_z\}$to the right-handed basis $\{\mathbf{f},\mathbf{g},\mathbf{f}\times\mathbf{g}\}$. The corresponding unitary operators, U_{R_P} and U_{R_Q}, perform the following transformations:

$$
\begin{aligned}
U_{R_P}XU_{R_P}^\dagger &= \boldsymbol{\sigma}\cdot R_P\mathbf{e}_x = \boldsymbol{\sigma}\cdot\mathbf{a} & \qquad U_{R_Q}XU_{R_Q}^\dagger &= \boldsymbol{\sigma}\cdot R_Q\mathbf{e}_x = \boldsymbol{\sigma}\cdot\mathbf{f} \\
U_{R_P}YU_{R_P}^\dagger &= \boldsymbol{\sigma}\cdot R_P\mathbf{e}_y = \boldsymbol{\sigma}\cdot\mathbf{c} & \qquad U_{R_Q}YU_{R_Q}^\dagger &= \boldsymbol{\sigma}\cdot R_Q\mathbf{e}_y = \boldsymbol{\sigma}\cdot\mathbf{g} \\
U_{R_P}ZU_{R_P}^\dagger &= \boldsymbol{\sigma}\cdot R_P\mathbf{e}_z = \boldsymbol{\sigma}\cdot\mathbf{a}\times\mathbf{c} & \qquad U_{R_Q}ZU_{R_Q}^\dagger &= \boldsymbol{\sigma}\cdot R_Q\mathbf{e}_z = \boldsymbol{\sigma}\cdot\mathbf{f}\times\mathbf{g}
\end{aligned}
\quad . \tag{3}
$$

It is easy to see that

$$
\begin{aligned}
(X\otimes X)U^\dagger_{R_P}\otimes U^\dagger_{R_Q}|\Psi\rangle &= (U^\dagger_{R_P}\otimes U^\dagger_{R_Q})(U_{R_P}XU^\dagger_{R_P}\otimes U_{R_Q}XU^\dagger_{R_Q})|\Psi\rangle \\
&= (U^\dagger_{R_P}\otimes U^\dagger_{R_Q})(\boldsymbol{\sigma}\cdot\mathbf{a}\otimes\boldsymbol{\sigma}\cdot\mathbf{f})|\Psi\rangle \\
&= \pm U^\dagger_{R_P}\otimes U^\dagger_{R_Q}|\Psi\rangle\ ,
\end{aligned}
\tag{4}
$$

i.e., that $U^\dagger_{R_P}\otimes U^\dagger_{R_Q}|\Psi\rangle$ is a ±1 eigenstate of $X\otimes X$. Similarly, we have that

$$
(Y\otimes Y)U^\dagger_{R_P}\otimes U^\dagger_{R_Q}|\Psi\rangle = \pm U^\dagger_{R_P}\otimes U^\dagger_{R_Q}|\Psi\rangle\ , \tag{5}
$$

i.e., that $U^\dagger_{R_P}\otimes U^\dagger_{R_Q}|\Psi\rangle$ is a ±1 eigenstate of $Y\otimes Y$.

For the lower sign, we get the singlet state,

$$
U^\dagger_{R_P}\otimes U^\dagger_{R_Q}|\Psi\rangle = |\beta_{11}\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)\ , \tag{6}
$$

and for the upper sign,

$$
U^\dagger_{R_P}\otimes U^\dagger_{R_Q}|\Psi\rangle = |\beta_{01}\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)\ . \tag{7}
$$

Both of these hold only up to a global phase, but that phase is irrelevant so we forget about it.

Our final conclusion is that is that the upper bound for the CHSH inequality is saturated if and only if

$$
|\Psi\rangle = \frac{1}{\sqrt{2}}\big(U_{R_P}|0\rangle\otimes U_{R_Q}|1\rangle \pm U_{R_P}|1\rangle\otimes U_{R_Q}|0\rangle\big)\ , \tag{8}
$$

with the measurements on the first qubit being along directions $\mathbf{a} = R_P\mathbf{e}_x$ and $\mathbf{c} = R_P\mathbf{e}_y$ and on the second qubit along directions $\mathbf{b} = (\mathbf{g}+\mathbf{f})/\sqrt{2} = R_Q(\mathbf{e}_y+\mathbf{e}_x)/\sqrt{2}$ and $\mathbf{d} = (\mathbf{g}-\mathbf{f})/\sqrt{2} = R_Q(\mathbf{e}_y-\mathbf{e}_x)/\sqrt{2}$. These results are local unitaries away from those we reached in class: the state has to be a maximally entangled state, with the measurement directions chosen to match the particular way the two qubits are correlated. We could dispense with the $\pm$ because one case can be converted into the other by absorbing a sign into the local unitaries, e.g., by preceding U_{R_P} by a 180° rotation about the z axis.

As a slightly nontrivial example, suppose both R_P and R_Q are -120° degree rotations about $(\mathbf{e}_x+\mathbf{e}_y+\mathbf{e}_z)/\sqrt{3}$. Such a rotation R permutes the axes according $R\mathbf{e}_x = \mathbf{e}_z$, $R\mathbf{e}_y = \mathbf{e}_x$, and $R\mathbf{e}_z = \mathbf{e}_y$. It can be decomposed into a 180° rotation about $(\mathbf{e}_x+\mathbf{e}_z)/\sqrt{2}$, whose corresponding unitary operator is the Hadamard transform $H = ie^{-i(X+Z)\pi/2\sqrt{2}} = (X+Z)/\sqrt{2}$, followed by a 90° rotation about $\mathbf{e}_z$, whose corresponding unitary operator is often denoted $S = e^{i\pi/4}e^{-iZ\pi/4}$ (the unit-determinant unitary operators for these rotations do not have the phase factors in front of the operator exponentials). These operators have the following matrix representations:

$$
H \to \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \qquad S \to \begin{pmatrix}1 & 0\\ 0 & i\end{pmatrix} \tag{9}
$$

Thus we have $U_{R_P} = U_{R_Q} = SH$. In this situation, the measurements are along $\mathbf{a} = R\mathbf{e}_x = \mathbf{e}_z$, $\mathbf{b} = R(\mathbf{e}_y + \mathbf{e}_x)/\sqrt{2} = (\mathbf{e}_x + \mathbf{e}_z)/\sqrt{2}$, $\mathbf{c} = R\mathbf{e}_y = \mathbf{e}_x$, and $\mathbf{d} = R(\mathbf{e}_y - \mathbf{e}_x)/\sqrt{2} = (\mathbf{e}_x - \mathbf{e}_z)/\sqrt{2}$, and the states that achieve the biggest violation of the CHSH inequality are

$$(S\otimes S)(H\otimes H)\frac{1}{\sqrt{2}}\big(|01\rangle \pm |10\rangle\big) = \begin{array}{c} S\otimes S(|00\rangle - |11\rangle)/\sqrt{2} \\ -S\otimes S(|01\rangle - |10\rangle)/\sqrt{2} \end{array} = \begin{array}{c} (|00\rangle + |11\rangle)/\sqrt{2} \\ -i(|01\rangle - |10\rangle)/\sqrt{2} \end{array} = \begin{array}{c} |\beta_{00}\rangle \\ -i|\beta_{11}\rangle \end{array}. \tag{10}$$

The singlet state (the overall phase of $-i$ is irrelevant) is one of the two possibilities, as is obvious from the start from its invariance under simultaneous rotations of both qubits.

For anyone who's interested, here's the old statement of the problem (drawn from Nielsen and Chuang Problem 2.3) and its solution.

3.x. **Maximal violation of the CHSH Bell inequality.** Let $A = \boldsymbol{\sigma}\cdot\mathbf{a}$, $B = \boldsymbol{\sigma}\cdot\mathbf{b}$, $C = \boldsymbol{\sigma}\cdot\mathbf{c}$, and $D = \boldsymbol{\sigma}\cdot\mathbf{d}$, where $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, and $\mathbf{d}$ are unit vectors in three dimensions, and let

$$\mathcal{B} = A\otimes B + C\otimes B + C\otimes D - A\otimes D = \boldsymbol{\sigma}\cdot\mathbf{a}\otimes\boldsymbol{\sigma}\cdot(\mathbf{b}-\mathbf{d}) + \boldsymbol{\sigma}\cdot\mathbf{c}\otimes\boldsymbol{\sigma}\cdot(\mathbf{b}+\mathbf{d})$$

be the *Bell operator*. The quantity we called S in our discussion of the CHSH inequality is the expectation value of the Bell operator, i.e., $S = \langle\mathcal{B}\rangle$.

(a) *Show* that

$$\mathcal{B}^2 = 4I\otimes I + [A,C]\otimes[B,D] = 4(I\otimes I - \boldsymbol{\sigma}\cdot\mathbf{a}\times\mathbf{c}\otimes\boldsymbol{\sigma}\cdot\mathbf{b}\times\mathbf{d})\ .$$

(b) Use the result of part (a) to *show* that

$$|\langle\mathcal{B}\rangle| \le 2\sqrt{2}\ .$$

This result, called *T'sirelson's inequality*, determines the maximal violation of the CHSH Bell inequality.

(c) *Find* the conditions for equality in T'sirelson's inequality. (Warning: This third part is hard, which is probably why it is not included in Nielsen and Chuang's Problem 2.3.)

3.x. $\mathcal{B} = A\otimes B + C\otimes B + C\otimes D - A\otimes D = \boldsymbol{\sigma}\cdot\mathbf{a}\otimes\boldsymbol{\sigma}\cdot(\mathbf{b}-\mathbf{d}) + \boldsymbol{\sigma}\cdot\mathbf{c}\otimes\boldsymbol{\sigma}\cdot(\mathbf{b}+\mathbf{d})$

(a) To get the first form of $\mathcal{B}^2$, all we need is that the square of any spin component is the unit operator, i.e., $A^2 = B^2 = C^2 = D^2 = I$. The rest is simply writing things out:

$$\begin{aligned}
\mathcal{B}^2 = {} & A^2\otimes B^2 + C^2\otimes B^2 + C^2\otimes D^2 + A^2\otimes D^2 \\
& + AC\otimes B^2 + CA\otimes B^2 - A^2\otimes BD - A^2\otimes DB \\
& + C^2\otimes BD + C^2\otimes DB - CA\otimes D^2 - AC\otimes D^2 \\
& + AC\otimes BD + CA\otimes DB - CA\otimes BD - AC\otimes DB \\
= {} & 4I\otimes I \\
& + (AC+CA)\otimes I - I\otimes(BD+DB) + I\otimes(BD+DB) - (CA+AC)\otimes I \\
& + AC\otimes[B,D] - CA\otimes[B,D] \\
= {} & 4I\otimes I + [A,C]\otimes[B,D]
\end{aligned} \tag{11}$$

Now recall that the product of two spin components is

$$AC = (\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{c}) = \sigma_j\sigma_k a_j c_k = (\delta_{jk} + i\epsilon_{jkl}\sigma_l)a_j c_k = a_j c_j + i\sigma_l\epsilon_{ljk}a_j c_k = \mathbf{a}\cdot\mathbf{c} + i\boldsymbol{\sigma}\cdot\mathbf{a}\times\mathbf{c}\ , \tag{12}$$

which gives us

$$\begin{aligned}
AC + CA &= 2\mathbf{a}\cdot\mathbf{c}\ , \\
[A,C] = AC - CA &= 2i\boldsymbol{\sigma}\cdot\mathbf{a}\times\mathbf{c}\ .
\end{aligned} \tag{13}$$

Plugging this into the expression for $\mathcal{B}^2$, we get the second form,

$$\mathcal{B}^2 = 4(I \otimes I - \boldsymbol{\sigma} \cdot \mathbf{a} \times \mathbf{c} \otimes \boldsymbol{\sigma} \cdot \mathbf{b} \times \mathbf{d}) \,. \tag{14}$$

(b) We start with the fact that for a Hermitian operator H,

$$\langle (\Delta H)^2 \rangle = \langle (H - \langle H \rangle)^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2 \,, \tag{15}$$

i.e.,

$$|\langle H \rangle|^2 = \langle H \rangle^2 = \langle H^2 \rangle - \langle (\Delta H)^2 \rangle \le \langle H^2 \rangle \,, \tag{16}$$

with equality if and only if the variance is zero, i.e., $\langle (\Delta H)^2 \rangle = 0$, which holds if and only if the state under consideration is an eigenstate of H. Let's apply this to the operator in part (a):

$$|\langle \mathcal{B} \rangle|^2 \le \langle \mathcal{B}^2 \rangle = 4 + \langle [A, C] \otimes [B, D] \rangle = 4(1 - \langle \boldsymbol{\sigma} \cdot \mathbf{a} \times \mathbf{c} \otimes \boldsymbol{\sigma} \cdot \mathbf{b} \times \mathbf{d} \rangle) \,. \tag{17}$$

Equality holds here if and only if $\langle \mathcal{B} \rangle^2 = \langle \mathcal{B}^2 \rangle$, i.e., the state under consideration is an eigenstate of $\mathcal{B}$.

Defining unit vectors $\mathbf{r}$ and $\mathbf{s}$ by $\mathbf{a} \times \mathbf{c} = |\mathbf{a} \times \mathbf{c}|\mathbf{r}$ and $\mathbf{b} \times \mathbf{d} = |\mathbf{b} \times \mathbf{d}|\mathbf{s}$, we can write

$$|\langle \mathcal{B} \rangle|^2 \le \langle \mathcal{B}^2 \rangle = 4\big(1 - |\mathbf{a} \times \mathbf{c}||\mathbf{b} \times \mathbf{d}| C(\mathbf{r}, \mathbf{s})\big) \,, \tag{18}$$

where $C(\mathbf{r}, \mathbf{s}) = \langle \boldsymbol{\sigma} \cdot \mathbf{r} \otimes \boldsymbol{\sigma} \cdot \mathbf{s} \rangle$ is the correlation coefficient between a measurement of $\boldsymbol{\sigma} \cdot \mathbf{r}$ on the first qubit and a measurement of $\boldsymbol{\sigma} \cdot \mathbf{s}$ on the second qubit. Since the spin components take on values ± 1, the correlation coefficient is bounded by $|C(\mathbf{r}, \mathbf{s})| \le 1$, which gives us

$$|\langle \mathcal{B} \rangle|^2 \le \langle \mathcal{B}^2 \rangle \le 4(1 + |\mathbf{a} \times \mathbf{c}||\mathbf{b} \times \mathbf{d}|) \tag{19}$$

with the second equality holding if and only if $C(\mathbf{r}, \mathbf{s}) = -1$, which is the same as saying the state is an eigenstate of $\boldsymbol{\sigma} \cdot \mathbf{r} \otimes \boldsymbol{\sigma} \cdot \mathbf{s}$ with eigenvalue -1.

Finally, using the fact the the magnitude of a cross product is bounded above by 1, we get

$$|\langle \mathcal{B} \rangle|^2 \le \langle \mathcal{B}^2 \rangle \le 4(1 + |\mathbf{a} \times \mathbf{c}||\mathbf{b} \times \mathbf{d}|) \le 8 \,, \tag{20}$$

which is the desired upper bound on $|\langle \mathcal{B} \rangle|$. Equality holds in the third inequality if and only if $|\mathbf{a} \times \mathbf{c}| = |\mathbf{b} \times \mathbf{d}| = 1$, which is the same as saying that $\mathbf{a}$ and $\mathbf{c}$ are at right angles and that $\mathbf{b}$ and $\mathbf{d}$ are at right angles.

(c) To achieve equality in the bound $|\langle \mathcal{B} \rangle|^2 \le 8$, we have to satisfy the three conditions listed above: (iii) $|\mathbf{a} \times \mathbf{c}| = |\mathbf{b} \times \mathbf{d}| = 1$, i.e., $\mathbf{a}$ and $\mathbf{c}$ are at right angles, and $\mathbf{b}$ and $\mathbf{d}$ are at right angles; (ii) $C(\mathbf{r}, \mathbf{s}) = -1$, i.e., the state is an eigenstate of $\boldsymbol{\sigma} \cdot \mathbf{r} \otimes \boldsymbol{\sigma} \cdot \mathbf{s}$ with eigenvalue -1; and (i) $\langle \mathcal{B} \rangle^2 = \langle \mathcal{B}^2 \rangle$, i.e., the state is an eigenstate of $\mathcal{B}$.

(iii) is easy to satisfy, so just do it. We have that $\{\mathbf{a}, \mathbf{c}, \mathbf{r} = \mathbf{a} \times \mathbf{c}\}$ and $\{\mathbf{b}, \mathbf{d}, \mathbf{s} = \mathbf{b} \times \mathbf{d}\}$ are right-handed sets of orthonormal vectors in three dimensions. Hence, $\{\mathbf{f} = (\mathbf{b} - \mathbf{d})/\sqrt{2}\,, \mathbf{g} = (\mathbf{b} + \mathbf{d})/\sqrt{2}\,, \mathbf{r} = \mathbf{f} \times \mathbf{g}\}$ is also a right-handed orthonormal set.

To satisfy (ii), we require that the quantum state $|\Psi\rangle$ satisfy

$$\boldsymbol{\sigma}\cdot\mathbf{r}\otimes\boldsymbol{\sigma}\cdot\mathbf{s}|\Psi\rangle = -|\Psi\rangle \ . \tag{21}$$

Once (ii) and (iii) have been satisfied, we have $\langle\mathcal{B}^2\rangle = 8$, so to satisfy (i) requires that

$$\pm 2\sqrt{2} = \langle\mathcal{B}\rangle = \sqrt{2}\big(\langle\boldsymbol{\sigma}\cdot\mathbf{a}\otimes\boldsymbol{\sigma}\cdot\mathbf{f}\rangle + \langle\boldsymbol{\sigma}\cdot\mathbf{c}\otimes\boldsymbol{\sigma}\cdot\mathbf{g}\rangle\big) \ . \tag{22}$$

The only way to satisfy this is to have both expectation values equal to $+1$ or -1 and the only way for this to be true is to have the quantum state be an eigenstate of both operators with the same eigenvalue, i.e,

$$\boldsymbol{\sigma}\cdot\mathbf{a}\otimes\boldsymbol{\sigma}\cdot\mathbf{f}|\Psi\rangle = \pm|\Psi\rangle \qquad \text{and} \qquad \boldsymbol{\sigma}\cdot\mathbf{c}\otimes\boldsymbol{\sigma}\cdot\mathbf{g}|\Psi\rangle = \pm|\Psi\rangle \ . \tag{23}$$

The easiest way to get a handle on what's going on is to introduce a rotation R_P that rotates the standard basis $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$ to the the right-handed basis $\{\mathbf{a}, \mathbf{c}, \mathbf{r}\}$ and another rotation R_Q that rotates the standard basis $\{\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z\}$to the right-handed basis $\{\mathbf{f}, \mathbf{g}, \mathbf{s}\}$. The corresponding unitary operators, U_{R_P} and U_{R_Q}, perform the following transformations:

$$\begin{aligned} U_{R_P} X U_{R_P}^\dagger &= \boldsymbol{\sigma}\cdot R_P\mathbf{e}_x = \boldsymbol{\sigma}\cdot\mathbf{a} \qquad & U_{R_Q} X U_{R_Q}^\dagger &= \boldsymbol{\sigma}\cdot R_Q\mathbf{e}_x = \boldsymbol{\sigma}\cdot\mathbf{f} \\ U_{R_P} Y U_{R_P}^\dagger &= \boldsymbol{\sigma}\cdot R_P\mathbf{e}_y = \boldsymbol{\sigma}\cdot\mathbf{c} \qquad & U_{R_Q} Y U_{R_Q}^\dagger &= \boldsymbol{\sigma}\cdot R_Q\mathbf{e}_y = \boldsymbol{\sigma}\cdot\mathbf{g} \ . \\ U_{R_P} Z U_{R_P}^\dagger &= \boldsymbol{\sigma}\cdot R_P\mathbf{e}_z = \boldsymbol{\sigma}\cdot\mathbf{r} \qquad & U_{R_Q} Z U_{R_Q}^\dagger &= \boldsymbol{\sigma}\cdot R_Q\mathbf{e}_z = \boldsymbol{\sigma}\cdot\mathbf{s} \end{aligned} \tag{24}$$

It is easy to see, for example, that

$$\begin{aligned} (Z\otimes Z)U_{R_P}^\dagger\otimes U_{R_Q}^\dagger|\Psi\rangle &= (U_{R_P}^\dagger\otimes U_{R_Q}^\dagger)(U_{R_P} Z U_{R_P}^\dagger\otimes U_{R_Q} Z U_{R_Q}^\dagger)|\Psi\rangle \\ &= (U_{R_P}^\dagger\otimes U_{R_Q}^\dagger)(\boldsymbol{\sigma}\cdot\mathbf{r}\otimes\boldsymbol{\sigma}\cdot\mathbf{s})|\Psi\rangle \\ &= -U_{R_P}^\dagger\otimes U_{R_Q}^\dagger|\Psi\rangle \ , \end{aligned} \tag{25}$$

i.e., that $U_{R_P}^\dagger\otimes U_{R_Q}^\dagger|\Psi\rangle$ is a -1 eigenstate of $Z\otimes Z$. Elaborating this, we have the following eigenvalue equations:

$$\begin{aligned} (X\otimes X)U_{R_P}^\dagger\otimes U_{R_Q}^\dagger|\Psi\rangle &= \pm U_{R_P}^\dagger\otimes U_{R_Q}^\dagger|\Psi\rangle \ , \\ (Y\otimes Y)U_{R_P}^\dagger\otimes U_{R_Q}^\dagger|\Psi\rangle &= \pm U_{R_P}^\dagger\otimes U_{R_Q}^\dagger|\Psi\rangle \ , \\ (Z\otimes Z)U_{R_P}^\dagger\otimes U_{R_Q}^\dagger|\Psi\rangle &= -U_{R_P}^\dagger\otimes U_{R_Q}^\dagger|\Psi\rangle \ . \end{aligned} \tag{26}$$

For the lower sign, we get the singlet state,

$$U_{R_P}^\dagger\otimes U_{R_Q}^\dagger|\Psi\rangle = |\beta_{11}\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |01\rangle) \ , \tag{27}$$

and for the upper sign,

$$U_{R_P}^\dagger \otimes U_{R_Q}^\dagger |\Psi\rangle = |\beta_{01}\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |01\rangle) \; . \tag{28}$$

Both of these hold only up to a global phase, but that phase is irrelevant to our conclusion.

Our final conclusion is that is that to saturate the upper bound for the CHSH inequality requires using one of the states

$$\frac{1}{\sqrt{2}}\big(U_{R_P}|0\rangle \otimes U_{R_Q}|1\rangle \pm U_{R_P}|1\rangle \otimes U_{R_Q}|0\rangle\big) \; , \tag{29}$$

and making measurements on the first qubit along directions $\mathbf{a} = R_P\mathbf{e}_x$ and $\mathbf{c} = R_P\mathbf{e}_y$ and on the second qubit along directions $\mathbf{b} = (\mathbf{g}+\mathbf{f})/\sqrt{2} = R_Q(\mathbf{e}_y + \mathbf{e}_x)/\sqrt{2}$ and $\mathbf{d} = (\mathbf{g}-\mathbf{f})/\sqrt{2} = R_Q(\mathbf{e}_y - \mathbf{e}_x)/\sqrt{2}$. These results are local unitaries away from those we reached in class: the state has to be a maximally entangled state, with the measurement directions chosen to match the particular way the two qubits are correlated. We could dispense with the $\pm$ because the minus sign can be absorbed into one of the local unitaries. Since we consistently used necessary and sufficient conditions for saturating the T'sirelson bound, our result is both necessary and sufficient for equality.

As a slightly nontrivial example, suppose both R_P and R_Q are $-120°$ degree rotations about $(\mathbf{e}_x+\mathbf{e}_y+\mathbf{e}_z)/\sqrt{3}$. Such a rotation R permutes the axes according $R\mathbf{e}_x = \mathbf{e}_z$, $R\mathbf{e}_y = \mathbf{e}_x$, and $R\mathbf{e}_z = \mathbf{e}_y$. It can be decomposed into a $180°$ rotation about $(\mathbf{e}_x + \mathbf{e}_z)/\sqrt{2}$, whose corresponding unitary operator is the Hadamard transform $H = ie^{-i(X+Z)\pi/2\sqrt{2}} = (X + Z)/\sqrt{2}$, followed by a $90°$ rotation about $\mathbf{e}_z$, whose corresponding unitary operator is often denoted $S = e^{i\pi/4}e^{-iZ\pi/4}$ (the unit-determinant unitary operators for these rotations do not have the phase factors in front of the operator exponentials). These operators have the following matrix representations:

$$H \to \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad S \to \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \tag{30}$$

(the unit-determinant unitary for a $90°$ rotation about Thus we have $U_{R_P} = U_{R_Q} = SH$. In this situation, the measurements are along $\mathbf{a} = R\mathbf{e}_x = \mathbf{e}_z$, $\mathbf{b} = R(\mathbf{e}_y+\mathbf{e}_x)/\sqrt{2} = (\mathbf{e}_x+\mathbf{e}_z)/\sqrt{2}$, $\mathbf{c} = R\mathbf{e}_y = \mathbf{e}_x$, and $\mathbf{d} = R(\mathbf{e}_y - \mathbf{e}_x)/\sqrt{2} = (\mathbf{e}_x - \mathbf{e}_z)/\sqrt{2}$, and the states that achieve the biggest violation of the CHSH inequality are

$$(S\otimes S)(H\otimes H)\frac{1}{\sqrt{2}}\big(|01\rangle \pm |10\rangle\big) = \begin{matrix} S\otimes S(|00\rangle - |11\rangle)/\sqrt{2} \\ -S\otimes S(|01\rangle - |10\rangle)/\sqrt{2} \end{matrix} = \begin{matrix} (|00\rangle + |11\rangle)/\sqrt{2} \\ -i(|01\rangle - |10\rangle)/\sqrt{2} \end{matrix} = \begin{matrix} |\beta_{00}\rangle \\ -i|\beta_{11}\rangle \end{matrix} \; . \tag{31}$$

The singlet state (the overall phase of $-i$ is irrelevant) is one of the two possibilities, as is obvious from the start from its invariance under simultaneous rotations of both qubits.