Quantum mechanics II, Chapter 2 : What makes quantum different

TA : Achille Mauri, Behrang Tafreshi, Gabriel Pescia, Manuel Rudolph, Reyhaneh Aghaei Saem, Ricard Puig, Sacha Lerch, Samy Conus, Tyson Jones

Sometimes observation kills.

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Problem 1 : Tsirelson's Bound

Suppose

$$Q = \mathbf{q} \cdot \sigma, \quad R = \mathbf{r} \cdot \sigma, \quad S = \mathbf{s} \cdot \sigma, \quad T = \mathbf{t} \cdot \sigma,$$

where $\mathbf{q}, \mathbf{r}, \mathbf{s}$ and $\mathbf{t}$ are real unit vectors in three dimensions. Let

$$A = Q \otimes S + R \otimes S + R \otimes T - Q \otimes T \tag{1}$$

Show that

$$A^2 = (Q \otimes S + R \otimes S + R \otimes T - Q \otimes T)^2 = 4I + [Q, R] \otimes [S, T].$$

Use this result to prove that

$$\langle A \rangle = \langle Q \otimes S \rangle + \langle R \otimes S \rangle + \langle R \otimes T \rangle - \langle Q \otimes T \rangle \leq 2\sqrt{2}.$$

What is the maximum value of $\langle A \rangle$ in the classical case ? What do you infer from the difference between the classical and the quantum result ?

Hint : Assume any classical observables Q, R, S, T with possible measurement outcomes ± 1. In classical physics all observables commute with each other.

We have the following observables

$$Q = \mathbf{q} \cdot \sigma, \quad R = \mathbf{r} \cdot \sigma, \quad S = \mathbf{s} \cdot \sigma, \quad T = \mathbf{t} \cdot \sigma, \tag{2}$$

where $\mathbf{q}, \mathbf{r}, \mathbf{s}$ and $\mathbf{t}$ are real unit vectors in three dimensions. Let

$$A = Q \otimes S + R \otimes S + R \otimes T - Q \otimes T. \tag{3}$$

We want to show that

$$A^2 = 4I + [Q, R] \otimes [S, T]. \tag{4}$$

First, consider the arbitrary observable of the form V.

$$V = \mathbf{v} \cdot \sigma \tag{5}$$

Here, it is shown that $V^2 = \mathbb{1}$,

$$V^2 = (\sum_i v_i \sigma_i)^2 = \sum_{i,j} v_i v_j \sigma_i \sigma_j = \sum_{i,j} v_i v_j (\delta_{ij}\mathbb{1} + i\varepsilon_{ijk}\sigma_k) \tag{6}$$

where we use the relations of the Pauli matrices and the fact that $\mathbf{v}$ is normal.

$$V^2 = (\sum_i v_i^2)\mathbb{1} = \mathbb{1} \tag{7}$$

Using this result, we can simplify A^2

$$\begin{aligned} A^2 = (Q\otimes S + R\otimes S + R\otimes T - Q\otimes T)^2 &= Q^2\otimes S^2 + QR\otimes S^2 + QR\otimes ST - Q^2\otimes ST \\ &\quad + RQ\otimes S^2 + R^2\otimes S^2 + R^2\otimes ST - RQ\otimes ST \\ &\quad + RQ\otimes TS + R^2\otimes TS + R^2\otimes T^2 - RQ\otimes T^2 \\ &\quad - Q^2\otimes TS - QR\otimes TS - QR\otimes T^2 + Q^2\otimes T^2 \\ &= \mathbb{1}\otimes\mathbb{1} + QR\otimes\mathbb{1} + QR\otimes ST - \mathbb{1}\otimes ST \\ &\quad + RQ\otimes\mathbb{1} + \mathbb{1}\otimes\mathbb{1} + \mathbb{1}\otimes ST - RQ\otimes ST \\ &\quad + RQ\otimes TS + \mathbb{1}\otimes TS + \mathbb{1}\otimes\mathbb{1} - RQ\otimes\mathbb{1} \\ &\quad - \mathbb{1}\otimes TS - QR\otimes TS - QR\otimes\mathbb{1} + \mathbb{1}\otimes\mathbb{1} \end{aligned}$$

By writing the non-unitary terms in the form of commutator, we get

$$\begin{aligned} A^2 &= 4\mathbb{1}\otimes\mathbb{1} + QR\otimes ST - RQ\otimes ST + RQ\otimes TS - QR\otimes TS \\ &= 4\mathbb{1}\otimes\mathbb{1} + (QR - RQ)\otimes(ST - TS) \\ &= 4\mathbb{1}\otimes\mathbb{1} + [Q,R]\otimes[S,T]. \end{aligned}$$

Now the problem asks to use this result to prove that

$$\langle Q\otimes S\rangle + \langle R\otimes S\rangle + \langle R\otimes T\rangle - \langle Q\otimes T\rangle \le 2\sqrt{2}. \tag{8}$$

So we need the expectation value of A. Using $\mathrm{Var}(A) = \langle A^2\rangle - \langle A\rangle^2 \ge 0$, we have

$$\langle A\rangle^2 \le \langle A^2\rangle, \tag{9}$$

where we use the fact that the variance of A is positive.

Now the last step is to upper bound $\langle A^2\rangle$.

$$\langle A^2\rangle = 4\langle\mathbb{1}\rangle + \langle[Q,R]\otimes[S,T]\rangle \tag{10}$$

where we use the linearity of the expectation value. To upper bound $\langle A^2\rangle$ we use the fact that it has four terms of the form $X\otimes Y$ (where X and Y are one-qubit operators with ± 1 eigenvalues) and the expectation value of each of them is less than one because their eigenvalues are all plus or minus one.

$$\langle A^2\rangle = 4 + \langle[Q,R]\otimes[S,T]\rangle \le 8 \tag{11}$$

More explicit :

$$[Q,R]\otimes[S,T] = (q_i r_j s_k t_l)\sigma_i\sigma_j\otimes\sigma_k\sigma_l + ... \tag{12}$$

Ignoring the coefficients and only taking the first term, we have :

$$\sigma_i \sigma_j \otimes \sigma_k \sigma_l = \delta_{ij} \otimes \delta_{kl} + i\epsilon_{ijm}\sigma_m \otimes \delta_{kl} + \delta_{ij} \otimes i\epsilon_{klm}\sigma m - \epsilon_{ijm}\sigma_m \otimes \epsilon_{kln}\sigma_n \tag{13}$$

Applying the above operator to a 2-particle state, computing the norm and using the triangle inequality gives :

$$\begin{aligned} |\sigma_i \sigma_j \otimes \sigma_k \sigma_l \,|\psi_1 \psi_2\rangle\,| \leq |\delta_{ij} \otimes \delta_{kl}\,|\psi_1 \psi_2\rangle\,| &\quad (14)\\ + |\sigma_m \otimes \delta_{kl}\,|\psi_1 \psi_2\rangle\,| &\quad (15)\\ + |\delta_{ij} \otimes \sigma_m\,|\psi_1 \psi_2\rangle\,| &\quad (16)\\ + |\sigma_m \otimes \sigma_n\,|\psi_1 \psi_2\rangle\,| &\quad (17)\end{aligned}$$

The point now is that in the above expression only one will contribute. For example if $i = j$ only the first or third term can contribute. Additionally if $k = l$ only the first contributes and if $k \neq l$ only the third contributes. Therefore the full expression is bounded from above by 1. Since there are 4 terms of the above form we have :

$$\langle A \rangle^2 \leq 8 \tag{18}$$

And by replacing A it can be written as follows

$$\langle Q \otimes S + R \otimes S + R \otimes T - Q \otimes T \rangle = \langle Q \otimes S \rangle + \langle R \otimes S \rangle + \langle R \otimes T \rangle - \langle Q \otimes T \rangle \leq 2\sqrt{2}. \tag{19}$$

Furthermore, it is crucial to show that this bound is attainable. Than can be done by giving a simple example. Let

$$\begin{aligned} Q =& \sigma_x &\quad (20)\\ R =& \sigma_z &\quad (21)\\ S =& -\frac{\sigma_z + \sigma_x}{\sqrt{2}} &\quad (22)\\ T =& \frac{\sigma_z - \sigma_x}{\sqrt{2}} &\quad (23)\\ & &\quad (24)\end{aligned}$$

Now prepare

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle\right) \tag{25}$$

and compute the expected values. It is easy to see that

$$\begin{aligned} \langle Q \otimes S \rangle_\psi =& \frac{1}{\sqrt{2}} &\quad (26)\\ \langle R \otimes S \rangle_\psi =& \frac{1}{\sqrt{2}} &\quad (27)\\ \langle R \otimes T \rangle_\psi =& \frac{1}{\sqrt{2}} &\quad (28)\\ \langle Q \otimes T \rangle_\psi =& \frac{-1}{\sqrt{2}} &\quad (29)\\ & &\quad (30)\end{aligned}$$

and thus

$$\langle Q \otimes S \rangle_\psi + \langle R \otimes S \rangle_\psi + \langle R \otimes T \rangle_\psi - \langle Q \otimes T \rangle_\psi = 2\sqrt{2} \tag{31}$$

For the classical case we have : $[Q, R] = [S, T] = 0$ and therefore $A \leq 2$. Using quantum resources, we can therefore violate the classical inequality by a factor of $\sqrt{2}$.

Problem 2 : Mermin-Peres and Telepathy

	1	**2**	**3**
1			
2			
3			

Figure 1 – Mermin-Peres Game Square

This exercise is another demonstration of quantum vs. classical correlations.
We consider Alice and Bob playing a cooperative game on a 3×3 square (see Figure 1). Alice will be assigned a secret row, and Bob assigned a secret column. The goal of the game is for Alice and Bob to fill their column/row with +1 or -1, without seeing each other's values, while respecting the following constraints :

- Alice's row must have an even number of -1 (None or 2) i.e. the product of the entries is +1.
- Bob's column must contain an odd number of -1 (1 or 3) i.e. the product of the entries is -1.
- The square which is in both, Alice's row and Bob's column, must be filled with the same number by both (both +1 or both -1).

Alice and Bob are allowed to strategize before the game, however any communication is forbidden after they have been assigned their respective row or column.

1. Suppose they only have access to classical resources. Find a strategy that works out with a probability of success of 8/9 (It can be shown that this is the optimal success probability using classical resources). *Hint : Try to fill as many squares as possible of the 3×3 square with +1 and -1, while respecting the given constraints. How many squares can you fill until you reach a contradiction ?*

Following the hint we start filling the empty squares with +1 and -1 until we reach a contradiction. This will inevitably happen for at least one square as can be seen below :

More systematically : gives :

	1	**2**	**3**
1	$+1$	$+1$	$+1$
2	$+1$	$+1$	$+1$
3	-1	-1	$-1/+1$

FIGURE 2 – Mermin-Peres Game Square

	1	**2**	**3**
1	a	b	c
2	d	e	f
3	g	h	i

FIGURE 3 – Mermin-Peres Game Square

$$
\begin{aligned}
a\,b\,c &= 1\\
d\,e\,f &= 1\\
g\,h\,i &= 1\\
a\,d\,g &= -1\\
b\,e\,h &= -1\\
c\,f\,i &= -1
\end{aligned}
$$

Multiplying the left-hand side of these six equations together gives $a^2\,b^2\,c^2\,d^2\,e^2\,f^2\,g^2\,h^2\,i^2 = 1$. But, multiplying the right-hand side together gives -1. So at most 8 of the table cells out of the 9 can be true.

2. What changes if Bob and Alice can communicate *after* learning the row/column they've been assigned ?

If they can communicate after leaving the room, they can share which row/column they are assigned. And thus they will win every time once again.

3. Now suppose Alice and Bob share two copies of a maximally entangled Bell state i.e. the full quantum state is $|\psi\rangle = \frac{1}{2}\left(|0000\rangle + |0011\rangle + |1100\rangle + |1111\rangle\right)$. Each of them has one part of the entangled state, and they can choose to perform on each spin a measurement of $\{X, Y, Z, \mathbb{1}\}$ (by "measuring $\mathbb{1}$" on spin i, it is meant that no measurement is performed on the i-th spin). The goal is to find a measurement strategy that beats the classical one in terms of success chances.

   Before the game starts, they start to think about a strategy to win the game and come up with the following idea :

	1	**2**	**3**
1	$+1/-1$	$+1$	$+1$
2	$+1$		
3	$+1$		

FIGURE 4 – Mermin-Peres Game Square after measuring $Z \otimes Z \otimes Z \otimes Z$ and obtaining $\{1,1,1,1\}$ as measurement outcome.

They want to agree upon measurements they can perform on their qubits, for every combination of row and column they could possibly get. If they find 9 measurements (for every combination of row and column) that will successfully fill their row and columns (successful means they agree in the ij-th square, while keeping their constraints), they would win the game always. They start trying out different measurments they could perform. For example : If Alice got row 1 and Bob got column 1 they would have to agree in the top left corner of the 3×3 square. They decide to try both measure Z on both their qubits i.e. they measure $Z \otimes Z \otimes Z \otimes Z$ on $|\psi\rangle$. This results in 4 different possibilities to fill the squares : If Alice and Bob both measure $\{1,1\}$, the state collapsed to $|0000\rangle$. Alice will put $\{1,1\}$ in the second and third square of the first row, and Bob will put $\{1,1\}$ in the second and third square of the first column. To respect the constraints Alice needs to fill another 1 in the top left square while Bob has to fill a -1 (see Figure 4). With this measurement they would therefore lose the game. Had they measured $\{1,1,-1,-1\}$ (corresponding to the collapse to $|0011\rangle$), Alice would fill again $\{1,1\}$ while Bob would fill $\{-1,-1\}$. Again respecting the constraints, Alice has to fill a 1, while Bob needs to fill a -1. They again lose.

Can you find a 4-qubit measurement that will result in a win every time, without failure ?

If they share a maximally entangled state they can win all the time. This is done by mapping the table in Figure 5. Crucially, every row (column) commutes, and thus they can be measured simultaneously. Suppose that the shared state looks like

$$|\Psi\rangle = \frac{1}{2}\left(|0_A 0_B 0_A 0_B\rangle + |0_A 0_B 1_A 1_B\rangle + |1_A 1_B 0_A 0_B\rangle + |1_A 1_B 1_A 1_B\rangle\right) \tag{32}$$

then if for example, A obtains row 1 and Bob obtains column 1, the complete measurement of the two would read : $\sigma_Z \otimes \sigma_X \otimes \sigma_Z \otimes \sigma_Z$ leading to the possible measurement outcomes $\{1_A, 1_B, 1_A, 1_B\}$, $\{1_A, -1_B, 1_A, 1_B\}$, $\{-1_A, 1_B, 1_A, 1_B\}$, $\{-1_A, -1_B, 1_A, 1_B\}$, $\{1_A, 1_B, -1_A, -1_B\}$, $\{1_A, -1_B, -1_A, -1_B\}$, $\{-1_A, 1_B, -1_A, -1_B\}$, $\{-1_A, -1_B, -1_A, -1_B\}$. Note that the results of Alice and Bob are fully correlated for what concerns the measurement of σ_z on the second pair of qubits. In other words, if Alice measures the value of σ_z on her second qubit and Bob measures σ_z on his second qubit, then in the entangled state $|\Psi\rangle$, they always get the same answer. Since in the top left corner Alice and Bob both write $1 \otimes \sigma_z$— that is, the value measured in their second qubit— they win the game with probability 1.

The same holds for any choice of row and column. Crucially, it is important that for each row (column) the measurements commute, and thus they can be measured simultaneously. You can check the **Wikipedia page** for more details.

	1	2	3	
1	$\mathbb{1} \otimes \sigma_z$	$\sigma_z \otimes \mathbb{1}$	$\sigma_z \otimes \sigma_z$	$+\mathbb{1}$
2	$\sigma_x \otimes \mathbb{1}$	$\mathbb{1} \otimes \sigma_x$	$\sigma_x \otimes \sigma_x$	$+\mathbb{1}$
3	$-\sigma_x \otimes \sigma_z$	$-\sigma_z \otimes \sigma_x$	$\sigma_y \otimes \sigma_y$	$+\mathbb{1}$
	$-\mathbb{1}$	$-\mathbb{1}$	$-\mathbb{1}$	

FIGURE 5 – Mermin-Peres Game Square

4. Do the same for every combination of rows and columns Alice and Bob can obtain.

If Alice obtains the first row she always measures σ_Z on both her particles. If she gets the second row she measures σ_X on both and if she gets the third row she measures σ_Y on both qubits. Bob measures $-\sigma_X \otimes \sigma_Z$ for the first, $-\sigma_Z \otimes \sigma_X$ for the second and $\sigma_Y \otimes \sigma_Y$ for the third column. Note that the product of the measurements along the columns gives $-\mathbb{1}$ while it is $\mathbb{1}$ along the rows. This was not possible using plain scalars.

Problem 3 : Bloch sphere for pure or mixed states of a two-level system

In the lecture you have started to talk about density matrices. This exercise serves as a first introduction to the topic, connecting to the already known concept of the Bloch sphere.

1. *Derivation of Bloch vector from generic pure state.* Any pure one-qubit quantum state can be written as ket

$$|\psi\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)e^{i\phi}|1\rangle \qquad \theta \in [0, \pi),\ \phi \in [0, 2\pi)$$

or as the density matrix,

$$|\psi\rangle\langle\psi| = \frac{1}{2}\left(\mathbb{1} + \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{r}\,\right)$$

Find an expression for $\mathbf{r}$ in terms of θ and ϕ. What does the vector $\mathbf{r}$ denote ?

We just have to expand the LHS and the RHS separately and then equate the matrix entries in a pairwise manner. Starting from the LHS, we have

$$|\psi\rangle\langle\psi| = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} \cos^2\frac{\theta}{2} & e^{-i\phi}\cos\frac{\theta}{2}\sin\frac{\theta}{2} \\ e^{i\phi}\cos\frac{\theta}{2}\sin\frac{\theta}{2} & \sin^2\frac{\theta}{2} \end{pmatrix}, \tag{33}$$

while for the RHS we have

$$\frac{1}{2}(\mathbb{1} + \boldsymbol{\sigma} \cdot \boldsymbol{r}) = \frac{1}{2}\begin{pmatrix} 1 + r_z & r_x - ir_y \\ r_x + ir_y & 1 - r_z \end{pmatrix}. \tag{34}$$

The diagonal entries yield the constraints $\cos^2\theta/2 = (1+r_z)/2$ and $\sin^2\theta/2 = (1-r_z)/2$, which can be subtracted to obtain

$$r_z = \cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2} = \cos\theta. \tag{35}$$

One can proceed similarly with the off-diagonal entries and find that by adding and subtracting the two associated equations, respectively, we get

$$r_x = \cos\frac{\theta}{2}\sin\frac{\theta}{2}(e^{-i\phi} + e^{i\phi}) = 2\cos\frac{\theta}{2}\sin\frac{\theta}{2}\cos\phi = \sin\theta\cos\phi, \tag{36}$$

$$r_y = \sin\theta\sin\phi. \tag{37}$$

So we recover the Bloch vector

$$\boldsymbol{r} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \tag{38}$$

which represents a unit vector in spherical coordinates in $\mathbb{R}^3$ (which is restricted to the boundary of the unit sphere).

2. *Derivation of Bloch vector from properties of density operators.* Define the set of density matrices with the following 3 conditions :
   - The density matrix is Hermitian : $\hat{\rho}^\dagger = \hat{\rho}$
   - It has trace 1 : $\mathrm{Tr}\hat{\rho} = 1$
   - It is positive or null : $\langle\Psi|\hat{\rho}|\Psi\rangle \geq 0, \quad \forall\Psi$

   Show that any density matrix $\hat{\rho}$ of the 2 level system can be written

$$\hat{\rho} = \frac{1}{2}(\mathbb{1} + \hat{\boldsymbol{\sigma}}\cdot\boldsymbol{r}), \tag{39}$$

   where $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$. Argue that $\boldsymbol{r}$ is a real vector of 3D space and $|\boldsymbol{r}| \leq 1$.

We know that density matrices are Hermitian. We also already showed in Problem Set 1 that any Hermitian operator ρ can be written as a linear combination of the Pauli matrices (including the identity operator), that is,

$$\rho = a\mathbb{1} + b\sigma_x + c\sigma_y + d\sigma_z = a\mathbb{1} + \boldsymbol{\sigma}\cdot\boldsymbol{r}', \tag{40}$$

where $a, b, c, d \in \mathbb{R}$, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ and $\boldsymbol{r'} = (b, c, d)$. Density matrices must additionally satisfy $\mathrm{Tr}\rho = 1$ and positivity, which yield the following contraints :

$$\mathrm{Tr}\rho = \mathrm{Tr}[a\mathbb{1}] = 2a = 1 \implies a = 1/2 \tag{41}$$

$$\tag{42}$$

and Eigenvalues have to be larger than 0. From (40) we have :

$$\rho = \begin{bmatrix} 1/2+d & b-ic \\ b+ic & 1/2-d \end{bmatrix} \tag{43}$$

$$\det[\lambda\mathbb{1} - \rho] = (\lambda - 1/2 - d)(\lambda - 1/2 + d) - b^2 - c^2 = 0 \tag{44}$$

$$= \lambda^2 - \lambda - |\mathbf{r}'|^2 + 1/4 \tag{45}$$

And therefore :

$$\lambda = 1/2 \pm |\mathbf{r}'| \geq 0 \tag{46}$$
$$|\mathbf{r}'| \leq 1/2 \tag{47}$$
$$|\mathbf{r}'| \geq -1/2 \tag{48}$$

All together we have $\rho = a\mathbb{1} + \mathbf{r}' \cdot \sigma = a\left(\mathbb{1} + \mathbf{r}'/a \cdot \sigma\right) = \frac{1}{2}\left(\mathbb{1} + \mathbf{r} \cdot \sigma\right)$ with $\mathbf{r} = 2\mathbf{r}'$ and $|\mathbf{r}| \leq 1$, as required.

Alternatively to the positivity one can also use $\mathrm{Tr}\{\rho^2\} \leq 1$, yielding :

$$\mathrm{Tr}\rho^2 = \mathrm{Tr}[a^2\mathbb{1} + 2a\boldsymbol{\sigma} \cdot \boldsymbol{r}' + (\boldsymbol{\sigma} \cdot \boldsymbol{r}')^2] = 2(a^2 + |\boldsymbol{r}'|^2), \tag{49}$$

where we used the fact that Pauli matrices are traceless, the linearity of the trace operation, and finally the rewriting $(\boldsymbol{\sigma} \cdot \boldsymbol{r}')^2 = \boldsymbol{r}' \cdot \boldsymbol{r}' \mathbb{1} + i(\boldsymbol{r}' \times \boldsymbol{r}')_k \sigma_k = |\boldsymbol{r}'|^2 \mathbb{1}$ (see Problem Set 1). Putting everything together we find

$$\frac{1}{2} + 2|\boldsymbol{r}'|^2 \leq 1 \quad \Longrightarrow \quad |\boldsymbol{r}'|^2 \leq \frac{1}{4} \quad \Longrightarrow \quad |\boldsymbol{r}| \leq 1, \tag{50}$$

provided $\boldsymbol{r}$ is chosen such that $\boldsymbol{r} = 2\boldsymbol{r}'$.

Notice that in the general case of mixed states, the Bloch vector can occupy the entire unit sphere – not just its boundary as for pure states.

3. Show that the state is pure iff $||\boldsymbol{r}|| = 1$. Explain why $\mathrm{Tr}[\rho^2]$ is a measure of the 'purity' of a quantum state.

Since it is a iff (if and only if statement), we must prove *both* directions of the condition. If we first assume that the state is pure, we have already seen in the first question, what the representation of the state is and that $|r| = 1$. Conversely, if we have $|r| = 1$ we know that we can represent any point on the surface of the unit sphere. Since after exercise 1, any point on the surface of the unit sphere is associated to a pure state, $|r| = 1$ implies that the state is pure.

Alternatively, for pure states we also have $\rho^2 = \rho$ (by definition in the first exercise), and therefore $\mathrm{Tr}\rho^2 = 1$, which means that the following condition must hold

$$\mathrm{Tr}\rho^2 = \mathrm{Tr}\left[\left(\frac{1}{2}(\mathbb{1} + \boldsymbol{\sigma} \cdot \boldsymbol{r})\right)^2\right] = \mathrm{Tr}\left[\frac{1}{4}\mathbb{1} + \frac{1}{4}|\boldsymbol{r}|^2\mathbb{1}\right] = \frac{1}{2} + \frac{1}{2}|\boldsymbol{r}|^2 = 1, \tag{51}$$

which is only satisfied when $|\boldsymbol{r}| = 1$. If on the other hand we assume that $|\boldsymbol{r}| = 1$, then from the formula above for $\mathrm{Tr}\rho^2$ we can directly conclude that necessarily the state is pure, that is, $\mathrm{Tr}\rho^2 = 1$.

$\mathrm{Tr}\rho^2$ is a good measure for purity because only pure states have $\mathrm{Tr}\rho^2 = 1$. For a fully mixed two-level state we have $\rho = \sum_i \frac{1}{2} |i\rangle \langle i|$ and therefore $\rho^2 = \sum_{i,j} \frac{1}{4} \sum_i |i\rangle \langle i|$ and $\mathrm{Tr}\rho^2 = \frac{1}{2}$.
In general for a Hilbert space of dimension d the maximally mixed state has $\mathrm{Tr}\rho^2 = 1/d$.

4. Sketch on the Bloch sphere the states :
a) $|0\rangle$
b) $|+\rangle := \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
c) $|-\rangle := \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

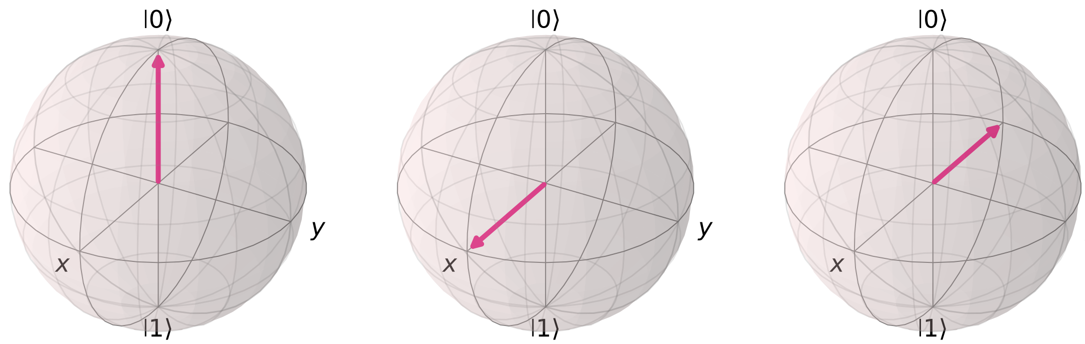
d) $\frac{1}{\sqrt{3}}(|0\rangle - i\sqrt{2}\,|1\rangle)$.
e) $\frac{1}{2}\mathbb{1}$
f) $\frac{1}{3}|+\rangle\langle+| + \frac{2}{3}|-\rangle\langle-|$

We employ the following two tricks to draw the one-qubit mixed states on the Bloch sphere :

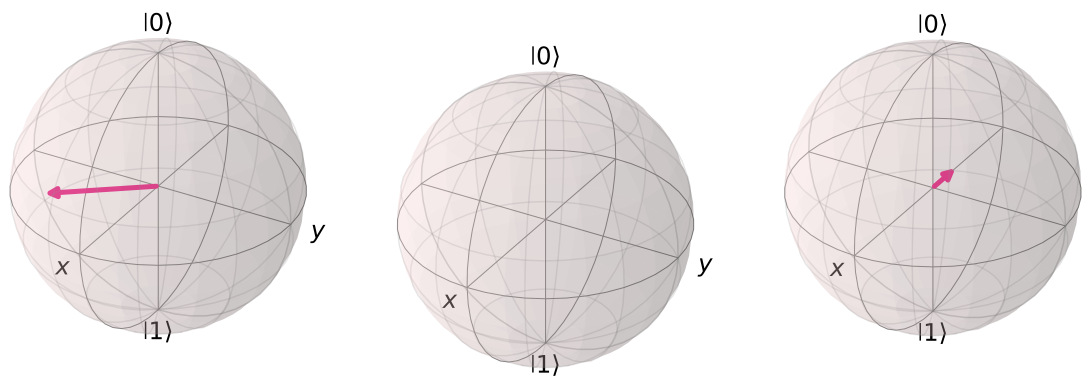
— A density matrix $\hat{\rho} = \frac{1}{2}(\mathbb{1} + \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{r})$ occupies the position $\boldsymbol{r}$ on the Bloch sphere (which we traditionally draw as a vector from the origin).

— A density matrix $\hat{\rho} = a\,\hat{\rho}_1 + b\,\hat{\rho}_2$, with respective vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, has a Bloch vector $\boldsymbol{r} = a\,\boldsymbol{r}_1 + b\,\boldsymbol{r}_2$.

In Fig. 6 we sketch the states on the Bloch sphere.



(a) $|0\rangle$, $\theta = 0$ and $\phi = 0$. (b) $|+\rangle$, $\theta = \pi/2$ and $\phi = 0$. (c) $|-\rangle$, $\theta = \pi/2$ and $\phi = \pi$.



(d) $(|0\rangle - i\sqrt{2}|1\rangle)/\sqrt{3}$, $\theta = 2\arccos(1/\sqrt{3})$ and $\phi = 3\pi/2$. (e) $\mathbb{1}/2$, $\boldsymbol{r} = (0,0,0)$. (f) $|+\rangle\langle+|/3 + 2|-\rangle\langle-|/3$, $\boldsymbol{r} = (-1/3, 0, 0)$.

FIGURE 6 – Bloch sphere representation on quantum states.

5. Give a geometric argument to show that $\frac{1}{2}(|+\rangle\langle+| + |-\rangle\langle-|) = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$. (Is this surprising ?)

   Disclaimer : think about the meaning of this state. How would you represent $|0\rangle\langle 0|$ on the Bloch sphere ? And $|1\rangle\langle 1|$? Now if the space of qubits is a convex space, what is the point in the Bloch sphere that represents the combination of the previous one ?

   Now make the same reasoning for $|+\rangle\langle +|$, $|-\rangle\langle -|$.

Notice that we have

$$\frac{1}{2}(|+\rangle\langle+| + |-\rangle\langle-|) = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{1}{2}\mathbb{1}, \tag{52}$$

which, as shown above, corresponds to the origin of the Bloch sphere, i.e. $\boldsymbol{r} = (0,0,0)$. This is expected since $\{|+\rangle, |-\rangle\}$ and $\{|0\rangle, |1\rangle\}$ both form a basis, and as seen from the Bloch sphere representation, they cancel out.
Also by definition of the ortho-normal basis :

$$\mathbb{1} = \sum_i |i\rangle\langle i| \tag{53}$$

$$U\mathbb{1}U^\dagger = \sum_i U|i\rangle\langle i|U^\dagger \tag{54}$$

$$\mathbb{1} = \sum_\alpha |\alpha\rangle\langle\alpha| \tag{55}$$

where U is the matrix describing a change of basis from span$\{|i\rangle\}$ to span$\{|\alpha\rangle\}$ (In this case from Z-basis to X-basis). So we have

$$\sum_i |i\rangle\langle i| = \mathbb{1} = \sum_\alpha |\alpha\rangle\langle\alpha|, \tag{56}$$

as desired.