PHYS-C0252 - Quantum Mechanics

Exercise set 1 - model solutions

Due date: May 1, 2024 by 23:59 on MyCourses
Return the exercises as a `.pdf`.
You can write by hand and take pictures, use digital note-taking or LaTeX etc.

1. Consider the vectors $|\psi\rangle = 4|\phi_1\rangle + i|\phi_2\rangle$ and $|\chi\rangle = 2|\phi_1\rangle + (1-4i)|\phi_2\rangle$, where $|\phi_1\rangle$ and $|\phi_2\rangle$ are orthonormal, i.e. $\langle\phi_k|\phi_m\rangle = \delta_{km}$, where $\delta_{km} = 1$ for $k = m$ and $\delta_{km} = 0$ for $k \neq m$.

   (a) Express $|\psi\rangle + |\chi\rangle$ and $\langle\psi| + \langle\chi|$ in their simplest form using $|\phi_1\rangle$ and $|\phi_2\rangle$.

   (b) Express $|\phi_1\rangle$ in terms of $|\psi\rangle$ and $|\chi\rangle$.

   (c) Calculate the inner products $\langle\psi|\chi\rangle$ and $\langle\chi|\psi\rangle$. Are they equal?

   (d) Show that $|\psi\rangle$ and $|\chi\rangle$ satisfy the Cauchy–Schwarz inequality and the triangle inequality.

Solution:

(a)

$$|\psi\rangle + |\chi\rangle = 4\,|\phi_1\rangle + i\,|\phi_2\rangle + 2\,|\phi_1\rangle + (1-4i)\,|\phi_2\rangle = 6\,|\phi_1\rangle + (1-3i)\,|\phi_2\rangle$$

$$\langle\psi| + \langle\chi| = 6\langle\phi_1| + (1+3i)\langle\phi_2|$$

(b)

$$\begin{aligned}
&x\,|\psi\rangle + y\,|\chi\rangle = |\phi_1\rangle \\
&\Leftrightarrow\ [4x+2y]\,|\phi_1\rangle + [ix + (1-4i)y]\,|\phi_2\rangle = |\phi_1\rangle \\
&\Leftrightarrow\ \begin{cases} 4x + 2y = 1 \\ ix + (1-4i)y = 0 \end{cases} \\
&\Leftrightarrow\ x = \frac{38+i}{170},\ y = \frac{9-2i}{170}
\end{aligned}$$

(c)

$$\begin{aligned}
&\langle\psi|\chi\rangle = 4\cdot 2\,\langle\phi_1|\phi_1\rangle + (-i)\cdot(1-4i)\,\langle\phi_2|\phi_2\rangle = 8 - 4 - i = 4 - i, \\
&\langle\chi|\psi\rangle = 4\cdot 2\,\langle\phi_1|\phi_1\rangle + (1+4i)\cdot i\,\langle\phi_2|\phi_2\rangle = 8 - 4 + i = 4 + i \\
&\qquad\Rightarrow \langle\psi|\chi\rangle = (\langle\chi|\psi\rangle)^* \neq \langle\chi|\psi\rangle.
\end{aligned}$$

Note that the result $\langle\psi|\chi\rangle = (\langle\chi|\psi\rangle)^*$ always holds for any two states $|\psi\rangle$ and $|\chi\rangle$. If $\langle\psi|\chi\rangle$ is real, this reduces to $\langle\psi|\chi\rangle = \langle\chi|\psi\rangle$.

(d)

$$|\langle\psi|\chi\rangle|^2 = (4)^2 + (1)^2 = 17$$
$$\langle\chi|\chi\rangle = (2)^2 + |1-4i|^2 = 4+1+16 = 21$$
$$\langle\psi|\psi\rangle = 4^2 + 1^2 = 17$$
$$\langle\psi|\psi\rangle\langle\chi|\chi\rangle = 17 \cdot 21 = 357$$

Thus

$$|\langle\psi|\chi\rangle|^2 < \langle\psi|\psi\rangle\langle\chi|\chi\rangle.$$

$$||\,|\psi\rangle + |\chi\rangle\,||^2 = \langle\psi|\psi\rangle + \langle\psi|\chi\rangle + \langle\chi|\psi\rangle + \langle\chi|\chi\rangle = 17 + 4 - i + 4 + i + 21 = 46$$
$$||\,|\psi\rangle + |\chi\rangle\,|| = \sqrt{46} \approx 6.8$$
$$||\psi|| + ||\chi|| = \sqrt{17} + \sqrt{21} \approx 8.7$$

Thus

$$||\,|\psi\rangle + |\chi\rangle|| \leq ||\psi|| + ||\chi||.$$

2. Consider the so-called Pauli operators $\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0|$, $\hat{\sigma}_y = -\mathrm{i}|0\rangle\langle 1| + \mathrm{i}|1\rangle\langle 0|$ and $\hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1|$, where $\{|0\rangle, |1\rangle\}$ form an orthonormal basis of the considered Hilbert space.

   (a) Show that each Pauli operator is Hermitian.

   (b) Write down the matrix representation of the Pauli operators. Hint: for an operator $\hat{A}$ and an orthonormal basis $\{|\phi_k\rangle\}_k$, the matrix element A_{jk} is defined as $\langle\phi_j|\hat{A}|\phi_k\rangle$.

   (c) Solve the eigenvalues and the corresponding eigenstates of each Pauli operator using the matrix form, and write the eigenstates using the ket vectors $|0\rangle$ and $|1\rangle$.

   (d) For each Pauli operator, show that the eigenstates are orthogonal.

Solution:

(a)

$$\begin{aligned}
\hat{\sigma}_x^\dagger &= (|0\rangle\langle 1| + |1\rangle\langle 0|)^\dagger = (|0\rangle\langle 1|)^\dagger + (|1\rangle\langle 0|)^\dagger \\
&= |1\rangle\langle 0| + |0\rangle\langle 1| = \hat{\sigma}_x \\
\hat{\sigma}_y^\dagger\dagger &= (-\mathrm{i}|0\rangle\langle 1|)^\dagger + (\mathrm{i}|1\rangle\langle 0|)^\dagger \\
&= \mathrm{i}|1\rangle\langle 0| - \mathrm{i}|0\rangle\langle 1| = \hat{\sigma}_y \\
\hat{\sigma}_z^\dagger\dagger &= (|0\rangle\langle 0|)^\dagger - (|1\rangle\langle 1|)^\dagger \\
&= |0\rangle\langle 0| - |1\rangle\langle 1| = \hat{\sigma}_z
\end{aligned}$$

(b) For any linear operator $\hat{A}$, we can express it in matrix form using the orthonormal basis $\{|\phi_n\rangle\}$ as

$$\hat{A} = \sum_{nm} A_{nm}|\phi_n\rangle\langle\phi_m|,$$

where A_{nm} is the matrix element of the operator $\hat{A}$, given by

$$A_{nm} = \langle\phi_n|\hat{A}|\phi_m\rangle.$$

Using the above, the matrix representation of the operator $\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0|$ in the basis $\{|0\rangle, |1\rangle\}$ has the matrix elements

$$(\sigma_x)_{00} = \langle 0|\hat{\sigma}_x|0\rangle = \langle 0|0\rangle\langle 1|0\rangle + \langle 0|1\rangle\langle 0|0\rangle = 0$$

$$(\sigma_x)_{01} = \langle 0|\hat{\sigma}_x|1\rangle = 1$$
$$(\sigma_x)_{10} = \langle 1|\hat{\sigma}_x|0\rangle = 1$$
$$(\sigma_x)_{11} = \langle 1|\hat{\sigma}_x|1\rangle = 0$$

Thus

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Similarly

$$\sigma_y = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}$$

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

(c) Starting from the eigenvalue equation, we have:

$$\hat{\sigma}_x|\psi\rangle = \lambda|\psi\rangle$$

$$(\hat{\sigma}_x - \lambda\hat{\mathrm{I}})|\psi\rangle = 0.$$

In matrix form, this is:

$$(\sigma_x - \lambda\mathrm{I})\psi = 0$$
$$\Rightarrow \det[\sigma_x - \lambda\mathrm{I}] = (1-\lambda)(-1-\lambda) = 0$$
$$\Rightarrow \lambda^2 - 1 = 0.$$

Thus $\lambda = \pm 1$. The eigenvalues of $\hat{\sigma}_y$ and $\hat{\sigma}_z$ can be obtained similarly, and they are also ± 1. The eigenstates can be obtained by plugging the eigenvalues into the eigenvalue equation. For example, for σ_y, suppose that the eigenvector corresponding to the eivenvalue +1 is

$$|\psi_y^+\rangle \hat{=} \begin{bmatrix} a \\ b \end{bmatrix}.$$

The eigenvalue equation in matrix form is then

$$\begin{aligned} \sigma_y \begin{bmatrix} a \\ b \end{bmatrix} &= +1 \cdot \begin{bmatrix} a \\ b \end{bmatrix} \\ \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} &= \begin{bmatrix} a \\ b \end{bmatrix} \\ \begin{bmatrix} -ib \\ ia \end{bmatrix} &= \begin{bmatrix} a \\ b \end{bmatrix}. \end{aligned}$$

This equivalent to the pair of equations:

$$\begin{cases} -ib & = a \\ ia & = b \end{cases}$$

Substitute $b = ia$ from the second equation to the first to find

$$-i \cdot (ia) = a \Rightarrow a = a,$$

so a can in fact be any complex number, and $b = ia$. So any vector of the form

$$\begin{bmatrix} a \\ ia \end{bmatrix} = a \cdot \begin{bmatrix} 1 \\ i \end{bmatrix}$$

is an eigenvector. For this to be normalized, we need to have

$$\begin{aligned} 1 &= \left(a \cdot \begin{bmatrix} 1 & i \end{bmatrix}\right)^* \cdot \left(a \cdot \begin{bmatrix} 1 \\ i \end{bmatrix}\right) = |a|^2 \cdot 2 \\ \Leftrightarrow a &= \frac{1}{\sqrt{2}}. \end{aligned}$$

Thus, the normalized eigenvector of σ_y corresponding to $\lambda = +1$ is

$$\psi_y^+ = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix},$$

which in the ket-vector form is

$$|\psi_y^+\rangle = \frac{|0\rangle + i\,|1\rangle}{\sqrt{2}}.$$

Using similar steps, we find the ket-vectors for the rest of the eigenstates:

$$|\psi_x^+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}, \quad |\psi_x^-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}},$$

$$|\psi_y^+\rangle = \frac{|0\rangle + \mathrm{i}|1\rangle}{\sqrt{2}}, \quad |\psi_y^-\rangle = \frac{|0\rangle - \mathrm{i}|1\rangle}{\sqrt{2}},$$
$$|\psi_z^+\rangle = |0\rangle, \quad |\psi_z^+\rangle = |1\rangle.$$

(d) For example, for $\hat{\sigma}_x$, we have

$$\langle\psi_x^+|\psi_x^-\rangle = \left(\frac{1}{\sqrt{2}}\right)^2 (\langle 0| + \langle 1|)\,(|0\rangle - |1\rangle) = \frac{1}{2}\Big(\underbrace{\langle 0|0\rangle}_{=1} + \underbrace{\langle 1|0\rangle}_{=0} - \underbrace{\langle 0|1\rangle}_{=0} - \underbrace{\langle 1|1\rangle}_{=1}\Big) = 0.$$

For $\hat{\sigma}_y$ and $\hat{\sigma}_z$ the results are similar. Note that $\langle\psi_y^+| = (\langle 0| - i\,\langle 1|)/\sqrt{2}$ because when flipping the bra to a ket you have to do the complex conjugation.

3. (a) Show that for a Hermitian bounded linear operator $\hat{H} : \mathcal{H} \to \mathcal{H}$, all of its eigenvalues are real and the eigenvectors corresponding to different eigenvalues are orthogonal. Hint: start by calculating $\langle\phi|\hat{H}|\phi\rangle$ for an eigenstate $|\phi\rangle$. In a similar fashion, show that the eigenvalues of an anti-Hermitian linear bounded operator $\hat{A} : \mathcal{H} \to \mathcal{H}$ are either purely imaginary or equal to zero. Note that for anti-Hermitian operators $\hat{A}$, we have $\hat{A}^\dagger = -\hat{A}$.

   (b) An important class of Hermitian operators is the *projectors*. Consider a Hilbert space $\mathcal{H}$ with an orthonormal basis $\{|\phi_i\rangle\}_{i\in I}$, where I is a suitable finite (or infinite) index set. A subset of these basis vectors $\{|\phi_j\rangle\}_{j\in J}$, where $J \subset I$ will form an orthonormal basis for a subspace $\mathcal{H}'$ of $\mathcal{H}$. Projector P onto the subspace $\mathcal{H}'$ is then defined as

$$P \equiv \sum_{j\in J} |\phi_j\rangle\,\langle\phi_j|\,.$$

   Show that P is indeed a Hermitian operator, and that it satisfies the equation $P^2 = P$.

   (c) Consider any linear bounded operator $\hat{B} : \mathcal{H} \to \mathcal{H}$

      i. Show that $\hat{B} - \hat{B}^\dagger$ is anti-Hermitian and $\hat{B} + \hat{B}^\dagger$ is Hermitian.

      ii. Show that $\hat{B}$ can be expressed as a linear combination of a Hermitian and an anti-Hermitian operator.

Solution:

(a) Let $|\phi\rangle$ be an eigenstate of $\hat{H}$ with eigenvalue λ, i.e., $\hat{H}\,|\phi\rangle = \lambda\,|\phi\rangle$. Then,

$$\langle\phi|\hat{H}|\phi\rangle = \left(|\phi\rangle\,, \hat{H}\,|\phi\rangle\right) = (|\phi\rangle\,, \lambda\,|\phi\rangle) = \lambda\,(|\phi\rangle\,, |\phi\rangle) = \lambda\,\langle\phi\mid\phi\rangle\,.$$

On the other hand,

$$\langle\phi|\hat{H}|\phi\rangle = \left(\hat{H}^\dagger\,|\phi\rangle\,, |\phi\rangle\right) = \left(\hat{H}\,|\phi\rangle\,, |\phi\rangle\right) = \lambda^*\,(|\phi\rangle\,, |\phi\rangle) = \lambda^*\,\langle\phi\mid\phi\rangle$$

$$\lambda = \lambda^* \Leftrightarrow \lambda \in \mathbb{R}.$$

Let λ_1 and λ_2 be two distinct eigenvalues of $\hat{H}$, with corresponding eigenstates $|\phi_1\rangle$, $|\phi_2\rangle$. Then,

$$\langle\phi_1|\hat{H}|\phi_2\rangle - \langle\phi_1|\hat{H}|\phi_2\rangle = 0.$$

$$\langle\phi_1|\hat{H}|\phi_2\rangle - \langle\phi_1|\hat{H}^\dagger|\phi_2\rangle = 0.$$
$$\langle\phi_1|\hat{H}|\phi_2\rangle - \langle\phi_2|\hat{H}|\phi_1\rangle^* = 0.$$
$$\lambda_2\langle\phi_1|\phi_2\rangle - \lambda_1^*\langle\phi_2|\phi_1\rangle^* = 0.$$
$$(\lambda_2 - \lambda_1)\langle\phi_1|\phi_2\rangle = 0,$$

where we have used $\hat{H}^\dagger = \hat{H}$ and $\lambda_1 \in \mathbb{R}$ based on the above. Then, if $\lambda_1 \neq \lambda_2$, we must have

$$\langle\phi_1|\phi_2\rangle = 0.$$

Let $\hat{A}|\phi\rangle = a|\phi\rangle$. Then, we have

$$\langle\phi|\hat{A}|\phi\rangle = \left(|\phi\rangle, \hat{A}\,|\phi\rangle\right) = (|\phi\rangle, a\,|\phi\rangle) = a\,\langle\phi|\phi\rangle\,.$$

On the other hand,

$$\langle\phi|\hat{A}|\phi\rangle = \left(\hat{A}^\dagger\,|\phi\rangle, |\phi\rangle\right) = \left(-\hat{A}\,|\phi\rangle, |\phi\rangle\right) = (-a\,|\phi\rangle, |\phi\rangle) = -a^*\,\langle\phi|\phi\rangle\,.$$

Thus,

$$a = -a^*.$$

(b)

$$\hat{P}^\dagger = \left(\sum_{j\in J}|\phi_j\rangle\langle\phi_j|\right)^\dagger = \sum_{j\in J}\left(|\phi_j\rangle\langle\phi_j|\right)^\dagger = \sum_{j\in J}|\phi_j\rangle\langle\phi_j| = \hat{P}.$$

$$\begin{aligned}\hat{P}^2 &= \sum_{j\in J}|\phi_j\rangle\langle\phi_j|\sum_{j'\in J}|\phi_{j'}\rangle\langle\phi_{j'}| = \sum_{j,j'\in J}|\phi_j\rangle\langle\phi_j|\phi_{j'}\rangle\langle\phi_{j'}| \\ &= \sum_{j,j'\in J}\delta_{j,j'}\,|\phi_j\rangle\langle\phi_{j'}| = \sum_j|\phi_j\rangle\langle\phi_j| = \hat{P}.\end{aligned}$$

(c) i.

$$(\hat{B} - \hat{B}^\dagger)^\dagger = \hat{B}^\dagger - (\hat{B}^\dagger)^\dagger.$$

Using $(B^\dagger)^\dagger = \hat{B}$,

$$(\hat{B} - \hat{B}^\dagger)^\dagger = \hat{B}^\dagger - \hat{B} = -(\hat{B} - \hat{B}^\dagger)$$

Thus, $\hat{B} - \hat{B}^\dagger$ is anti-Hermitian.

$$(\hat{B} + \hat{B}^\dagger)^\dagger = \hat{B}^\dagger + (\hat{B}^\dagger)^\dagger = \hat{B} + \hat{B}^\dagger$$

Therefore, $\hat{B} + \hat{B}^\dagger$ is Hermitian.

ii.

$$\hat{B} = \frac{\hat{B} + \hat{B}^\dagger}{2} + \frac{\hat{B} - \hat{B}^\dagger}{2}.$$

4. (a) Prove the Cauchy–Schwarz inequality $|\langle\psi|\phi\rangle| \leq ||\psi||\,||\phi||$. Here we use the shorthand notation $||\psi||$ (= $||\,|\psi\rangle||$) for the norm of $|\psi\rangle$ as on lectures. Hint: Start from $0 \leq ||\,|\psi\rangle + \lambda|\phi\rangle\,||$ and choose the scalar $\lambda \propto \langle\phi|\psi\rangle$ in a clever way.

   (b) Prove the triangle inequality $||\,|\psi\rangle + |\phi\rangle|| \leq ||\psi|| + ||\phi||$. Hint: Calculate $||\,|\psi\rangle + |\phi\rangle\,||^2$ and use (a). You may also use the fact that $\mathrm{Re}(z) \leq |z|$ for a complex number z.

   (c) Demonstrate the necessary and sufficient conditions for these inequalities to become equalities. Hint: Let $a\,|\psi\rangle = \frac{\langle\psi|\phi\rangle}{\langle\psi|\psi\rangle}\,|\psi\rangle$ be the *projection* of $|\phi\rangle$ on to $|\psi\rangle$. You can write $|\phi\rangle$ in terms of the projection and the *rejection* $|\chi\rangle = |\phi\rangle - \frac{\langle\psi|\phi\rangle}{\langle\psi|\psi\rangle}\,|\psi\rangle$ as $|\phi\rangle = a\,|\psi\rangle + |\chi\rangle$. Note that the rejection is orthogonal to $|\psi\rangle$, i.e. $\langle\chi|\psi\rangle = 0$.

Solution:

(a) From the definition of the inner product we know

$$0 \leq ||\,|\psi\rangle + \lambda|\phi\rangle\,||^2$$
$$\Rightarrow 0 \leq \langle\psi|\psi\rangle + \lambda\lambda^*\langle\phi|\phi\rangle + \lambda^*\langle\phi|\psi\rangle + \lambda\langle\psi|\phi\rangle.$$

Now let $\lambda = -\langle\phi|\psi\rangle/\langle\phi|\phi\rangle$. Then,

$$0 \leq \langle\psi|\psi\rangle + \frac{|\langle\psi|\phi\rangle|^2}{\langle\phi|\phi\rangle} - \frac{|\langle\psi|\phi\rangle|^2}{\langle\phi|\phi\rangle} - \frac{|\langle\psi|\phi\rangle|^2}{\langle\phi|\phi\rangle},$$
$$0 \leq \langle\psi|\psi\rangle - \frac{|\langle\psi|\phi\rangle|^2}{\langle\phi|\phi\rangle} = ||\psi||^2 - \frac{|\langle\psi|\phi\rangle|^2}{||\phi||^2},$$

where we have used $\langle v|v\rangle = ||v||^2$. Multiplying both sides by $||\phi||^2$ and rearranging terms, we arrive at the inequality:

$$|\langle\psi|\phi\rangle|^2 \leq ||\psi||^2\,||\phi||^2.$$

Since everything is positive, we can take the square root of both sides to obtain the Cauchy-Schwarz inequality.

(b)

$$\begin{aligned}||\,|\psi\rangle + |\phi\rangle\,||^2 &= \langle\psi|\psi\rangle + \langle\phi|\phi\rangle + \langle\phi|\psi\rangle + \langle\psi|\phi\rangle \\ &= \langle\psi|\psi\rangle + 2\mathrm{Re}(\langle\phi|\psi\rangle) + \langle\phi|\phi\rangle\end{aligned}$$

For any complex number z, $\mathrm{Re(z)} \leq |\mathrm{z}|$. Thus

$$||\,|\psi\rangle + |\phi\rangle\,||^2 \leq ||\psi||^2 + 2|\langle\phi|\psi\rangle| + ||\phi||^2$$

Using the Cauchy–Schwarz inequality, we obtain

$$||\,|\psi\rangle + |\phi\rangle\,||^2 \leq ||\psi||^2 + 2||\psi||\,||\phi|| + ||\phi||^2 = (||\psi|| + ||\phi||)^2$$

Taking the square root of both sides yields the triangle inequality.

(c) If either $|\psi\rangle$ or $|\phi\rangle$ are the zero vector, the equality holds trivially. Let us then assume both are nonzero. Consider the rejection of $|\phi\rangle$ from $|\psi\rangle$, defined as $|\chi\rangle = a|\psi\rangle + |\phi\rangle$, where $a = -\langle\phi|\psi\rangle / \langle\psi|\psi\rangle$.

To avoid computing it again every time we need it, we first note that

$$\begin{aligned}||\phi|| &= \sqrt{\langle\phi|\phi\rangle} = \sqrt{||a|\psi\rangle + |\chi\rangle\,||} = \sqrt{|a|^2\langle\psi|\psi\rangle + \langle\psi|\chi\rangle + \langle\chi|\psi\rangle + \langle\chi|\chi\rangle} \\ &= \sqrt{|a|^2||\psi||^2 + ||\chi||^2},\end{aligned}$$

since $|\psi\rangle$ and $|\chi\rangle$ are orthogonal. You may recognize the property

$$||\,|a\rangle + |b\rangle\,||^2 = ||a||^2 + ||b||^2,$$

when $|a\rangle$ and $|b\rangle$ are orthogonal, as the (generalized) *Pythagorean theorem*.

Cauchy-Schwartz
Assume that the Cauchy-Schwartz equality holds:

$$|\langle\psi|\phi\rangle| = ||\psi||\,||\phi||.$$

Then (using the Pythagorean theorem for $||\phi||$),

$$\begin{aligned}|\langle\psi|\,(a|\psi\rangle + |\chi\rangle)| &= ||\psi|| \cdot \sqrt{|a|^2||\psi||^2 + ||\chi||^2} \\ \Leftrightarrow |a|\,\langle\psi|\psi\rangle &= ||\psi|| \cdot \sqrt{|a|^2||\psi||^2 + ||\chi||^2} \\ \Leftrightarrow |a|^2\,\langle\psi|\psi\rangle^2 &= ||\psi||^2 \cdot (|a|^2||\psi||^2 + ||\chi||^2) \\ \Leftrightarrow |a|^2||\psi||^4 &= ||\psi||^2 \cdot (|a|^2||\psi||^2 + ||\chi||^2) \\ \Leftrightarrow |a|^2||\psi||^2 &= |a|^2||\psi||^2 + ||\chi||^2 \\ \Leftrightarrow ||\chi||^2 &= 0 \\ \Leftrightarrow |\chi\rangle &= 0.\end{aligned}$$

So the necessary and sufficient condition for the C-S inequality to become an equality is that the rejection is zero, that is

$$|\phi\rangle = a|\psi\rangle\,,\ a \in \mathbb{C}.$$

Approach 2 for the C-S equality: Writing $|\phi\rangle$ in terms of $|\chi\rangle$ and $|\psi\rangle$ as before,

we have

$$||\phi||^2 = \|\chi\|^2 + |a|^2\|\psi\|^2.$$

Now, we note that

$$|a|^2 = \left|\frac{\langle\phi|\psi\rangle}{\langle\psi|\psi\rangle}\right|^2 = \frac{|\,\langle\phi|\psi\rangle\,|^2}{\|\psi\|^4}.$$

Now, if we assume that the Cauchy-Schwarz inequality is in fact an equality, we have $|\langle\phi|\psi\rangle|^2 = \|\psi\|^2\|\phi\|^2$, and thus

$$|a|^2 = \frac{\|\psi\|^2\|\phi\|^2}{\|\psi\|^4} = \frac{\|\phi\|^2}{\|\psi\|^2}.$$

If we now plug this into the earlier expression for $||\phi||^2$, we find

$$\|\phi\|^2 = \|\chi\|^2 + \frac{\|\phi\|^2}{\|\psi\|^2}\|\psi\|^2 = \|\chi\|^2 + \|\phi\|^2.$$

This can hold only if $\|\chi\| = 0$.

Triangle equality:

Let's assume the inequality is an equality: (

$$\begin{aligned}
||\,|\psi\rangle + |\phi\rangle\,|| &= ||\psi|| + ||\phi|| \\
\Leftrightarrow ||\,|\psi\rangle + |\phi\rangle\,||^2 &= ||\psi||^2 + ||\phi||^2 + 2||\psi||\cdot||\phi|| \\
\Leftrightarrow ||\psi||^2 + \langle\psi|\phi\rangle + \langle\phi|\psi\rangle + ||\phi||^2 &= ||\psi||^2 + ||\phi||^2 + 2||\psi||\cdot||\phi|| \\
\Leftrightarrow \langle\psi|\phi\rangle + \langle\phi|\psi\rangle &= 2||\psi||\cdot||\phi|| \\
\Leftrightarrow \langle\psi|\,(a\,|\psi\rangle + |\chi\rangle) + (a^*\,\langle\psi| + \langle\chi|)\,|\psi\rangle &= 2||\psi||\cdot||\phi|| \\
\Leftrightarrow a||\psi||^2 + a^*||\psi||^2 &= 2||\psi||\cdot||\phi|| \\
\Leftrightarrow (a + a^*)||\psi|| &= 2||\phi|| \\
\Leftrightarrow ||\phi|| &= \frac{a + a^*}{2}||\psi|| = \mathrm{Re}\{a\}||\psi||,
\end{aligned}$$

where $\mathrm{Re}\{a\}$ is the real part of a $\left(a = x + iy \rightarrow \frac{a+a^*}{2} = \frac{x+iy+x-iy}{2} = x = \mathrm{Re}\{a\}\right)$. Writing $||\phi||$ using the Pythagorean theorem and taking the square, we then have

$$\begin{aligned}
|a|^2||\psi||^2 + ||\chi||^2 &= \mathrm{Re}\{a\}^2||\psi||^2 \\
\Leftrightarrow \left(\mathrm{Re}\{a\}^2 + \mathrm{Im}\{a\}^2\right)||\psi||^2 + ||\chi||^2 &= \mathrm{Re}\{a\}^2||\psi||^2 \\
\mathrm{Im}\{a\}^2 &= -||\chi||^2
\end{aligned}$$

Since the left side is always positive or zero and the right side is always negative or zero, this suggests

$$||\chi|| = 0,\ \mathrm{Im}\{a\} = 0.$$

Thus the necessary and sufficient condition for the triangle inequality to become an equality is that the rejection is zero and that $|\phi\rangle$ is *parallel* to $|\psi\rangle$, that is

$$|\phi\rangle = a\,|\psi\rangle\,,\ a \in \mathbb{R}.$$