Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

Blatt 6

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Das Übungsblatt wird in Gruppen von maximal 3 Personen bearbeitet. Die Abgabe erfolgt digital über ILIAS.

Aufgabe 1. (Punkte)

Lösung Aufgabe 1.

1. To show that $(\hat{A}\,|\psi\rangle)^\dagger = \langle\psi|\,\hat{A}^\dagger$ it suffices to show that $(\hat{A}\,|\psi\rangle)^\dagger\,|\theta\rangle = \langle\psi|\hat{A}^\dagger|\theta\rangle$ for all $|\theta\rangle \in \mathcal{H}$. So, setting $\hat{A}\,|\psi\rangle = |\nu\rangle$ for convenience, then:

$$(\hat{A}\,|\psi\rangle)^\dagger\,|\theta\rangle = (|\nu\rangle)^\dagger\,|\theta\rangle = \langle\nu|\theta\rangle = \big(\,\langle\theta|\nu\rangle\,\big)^* = \big(\,\langle\theta|\hat{A}|\psi\rangle\,\big)^* = \Big(\big(\,\langle\psi|\hat{A}^\dagger|\theta\rangle\,\big)^*\Big)^* = \langle\psi|\hat{A}^\dagger|\theta\rangle \Rightarrow (\hat{A}\,|\psi\rangle)^\dagger = \langle\psi|\,\hat{A}^\dagger$$

2. Pick any $|\psi\rangle\,, |\theta\rangle \in \mathcal{H}$, then:

$$\langle\psi|\hat{A}|\theta\rangle = \big(\,\langle\theta|\hat{A}^\dagger|\psi\rangle\,\big)^* = \Big(\big(\,\langle\psi|(\hat{A}^\dagger)^\dagger|\theta\rangle\,\big)^*\Big)^* = \langle\psi|(\hat{A}^\dagger)^\dagger|\theta\rangle \Rightarrow (\hat{A}^\dagger)^\dagger = \hat{A}$$

3. Pick any $|\psi\rangle\,, |\theta\rangle \in \mathcal{H}$, then:

$$\langle\psi|(\alpha\hat{A})^\dagger|\theta\rangle = \big(\,\langle\theta|\alpha\hat{A}|\psi\rangle\,\big)^* = \alpha^*\big(\,\langle\theta|\hat{A}|\psi\rangle\,\big)^* = \alpha^*\,\langle\psi|\hat{A}^\dagger|\theta\rangle = \langle\psi|\alpha^*\hat{A}^\dagger|\theta\rangle \Rightarrow (\alpha\hat{A})^\dagger = \alpha^*\hat{A}^\dagger$$

4. Pick any $|\psi\rangle\,, |\theta\rangle \in \mathcal{H}$, then:

$$\begin{aligned}\langle\psi|(\hat{A}+\hat{B})^\dagger|\theta\rangle &= \big(\,\langle\theta|\hat{A}+\hat{B}|\psi\rangle\,\big)^* = \big(\,\langle\theta|\hat{A}|\psi\rangle + \langle\theta|\hat{B}|\psi\rangle\,\big)^* = \big(\,\langle\theta|\hat{A}|\psi\rangle\,\big)^* + \big(\,\langle\theta|\hat{B}|\psi\rangle\,\big)^* \\ &= \langle\psi|\hat{A}^\dagger|\theta\rangle + \langle\psi|\hat{B}^\dagger|\theta| = \langle\psi|\hat{A}^\dagger + \hat{B}^\dagger|\theta\rangle \Rightarrow (\hat{A}+\hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger\end{aligned}$$

5. Pick any $|\psi\rangle\,, |\theta\rangle \in \mathcal{H}$. Set $\langle\theta|\,\hat{A} = \langle\nu|$ and $\hat{B}\,|\psi\rangle = |\eta\rangle$. Then:

$$\langle\psi|(\hat{A}\hat{B})^\dagger|\theta\rangle = \big(\,\langle\theta|\hat{A}\hat{B}|\psi\rangle\,\big)^* = \big(\,\langle\nu|\eta\rangle\,\big)^* = \langle\eta|\nu\rangle = \big(\hat{B}\,|\psi\rangle\,\big)^\dagger\big(\,\langle\theta|\,\hat{A}\big)^\dagger = \langle\psi|\hat{B}^\dagger\hat{A}^\dagger|\theta\rangle \Rightarrow (\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$$

Aufgabe 2. Eigenschaften der Spur (? Punkte)

Gegeben sei ein Hilbertraum $\mathcal{H}$ mit endlicher Dimension d, ein linearer Operator $\hat{A}$, der auf $\mathcal{H}$ wirkt, und eine orthonormale Basis $\{|\psi_n\rangle\} \in \mathcal{H}$ mit $n = 1, \ldots, d$. Wir können die Spur von $\hat{A}$ in dieser orthogonalen Basis definieren als

$$\mathrm{tr}_\psi[\hat{A}] = \sum_{n=1}^{d} \langle\psi_n|\hat{A}|\psi_n\rangle\,.$$

1. Zeigen Sie für beliebige Operatoren $\hat{A}, \hat{B}$, dass

$$\mathrm{tr}_\psi[\hat{A}\hat{B}] = \mathrm{tr}_\psi[\hat{B}\hat{A}].$$

Verwenden Sie dieses Ergebnis, um zu zeigen, dass

$$\mathrm{tr}_\psi[\hat{A}\hat{B}\hat{C}] = \mathrm{tr}_\psi[\hat{C}\hat{A}\hat{B}] = \mathrm{tr}_\psi[\hat{B}\hat{C}\hat{A}].$$

Diese Eigenschaft ist die Invarianz der Spur unter zyklischen Vertauschungen. Wir können die Produkte in der Spur nicht beliebig permutieren, aber wir können sie vom Ende and das Anfang der Spur verschieben.

2. Definieren Sie den Basiswechseloperator $\hat{E}^\theta_\psi = \sum_{n=1}^d |\psi_n\rangle\langle\theta_n|$ wobei $\{|\psi_n\rangle\}$ und $\{|\theta_n\rangle\}$ zwei orthonormale Basen von $\mathcal{H}$ sind. Berechnen Sie dann das Inverse von $\hat{E}^\theta_\psi$ und zeigen Sie, dass $(\hat{E}^\theta_\psi)^{-1} = \hat{E}^\psi_\theta$, d.h., dass $\hat{E}^\theta_\psi\hat{E}^\psi_\theta = \mathbb{1}$. Welche Art Operator ist $\hat{E}^\theta_\psi$? Zeigen Sie schließlich, dass dieser Operator tatsächlich eine Basisänderung bewirkt, d.h. zeigen Sie, dass $\langle\psi_j|\hat{A}|\psi_k\rangle = \langle\theta_j|\hat{E}^\psi_\theta\hat{A}\hat{E}^\theta_\psi|\theta_k\rangle$.

3. Gegeben seien wieder $\{|\psi_n\rangle\}$ und $\{|\theta_n\rangle\}$ als orthonormale Basen von $\mathcal{H}$. Definieren Sie die Spur über die $\{|\psi_n\rangle\}$-Basis wie in der Einleitung und definieren sie die Spur über die $\{|\theta_n\rangle\}$-Basis als $\mathrm{tr}_\theta[\hat{A}] = \sum_{n=1}^d \langle\theta_n|\hat{A}|\theta_n\rangle$. Zeigen Sie für einen beliebigen Operator $\hat{A}$, dass

$$\mathrm{tr}_\psi[\hat{A}] = \mathrm{tr}_\theta[\hat{A}].$$

Die Spur ist also unabhängig von der gewählten Orthonormalbasis. Wir verwenden die basisunabhängige Notation $\mathrm{tr}[\hat{A}]$.

4. In der Vorlesung wurde die kanonische Kommutatorrelation $[\hat{x}, \hat{p}] = i\hbar\mathbb{1}$ für Orts- und Impulsoperator eingeführt. Benutzen Sie die Kommutatorrelation und die Eigenschaften der Spur, um zu zeigen, dass es nicht möglich ist, Orts- und Impulsoperatoren zu definieren als Operatoren, die auf einen endlichdimensionalen Hilbertraum wirken.

Lösung Aufgabe 2.

1. Zunächst demonstrieren wir, dass $\mathrm{tr}_\psi[\hat{A}\hat{B}] = \mathrm{tr}_\psi[\hat{B}\hat{A}]$:

$$\begin{aligned}
\mathrm{tr}_\psi[\hat{A}\hat{B}] &= \sum_{n=1}^d \langle\psi_n|\hat{A}\hat{B}|\psi_n\rangle = \sum_{n=1}^d\sum_{m=1}^d \langle\psi_n|\hat{A}|\psi_m\rangle\langle\psi_m|\hat{B}|\psi_n\rangle \quad \text{insert identity: } \mathbb{1} = \sum_{m=1}^d |\psi_m\rangle\langle\psi_m| \\
&= \sum_{n=1}^d\sum_{m=1}^d \langle\psi_m|\hat{B}|\psi_n\rangle\langle\psi_n|\hat{A}|\psi_m\rangle = \sum_{m=1}^d \langle\psi_m|\hat{B}\hat{A}|\psi_m\rangle \quad \text{remove identity: } \mathbb{1} = \sum_{n=1}^d |\psi_n\rangle\langle\psi_n| \\
&= \mathrm{tr}_\psi[\hat{B}\hat{A}].
\end{aligned}$$

Nun können wir dieses Ergebnis benutzen, um die zyklische Eigenschaft der Spur zu beweisen:

$$\begin{aligned}
\mathrm{tr}_\psi[\hat{A}\hat{B}\hat{C}] &= \mathrm{tr}_\psi[(\hat{A}\hat{B})\hat{C}] = \mathrm{tr}_\psi[\hat{C}(\hat{A}\hat{B})] = \mathrm{tr}_\psi[\hat{C}\hat{A}\hat{B}] \\
\mathrm{tr}_\psi[\hat{A}\hat{B}\hat{C}] &= \mathrm{tr}_\psi[\hat{A}(\hat{B}\hat{C})] = \mathrm{tr}_\psi[(\hat{B}\hat{C})\hat{A}] = \mathrm{tr}_\psi[\hat{B}\hat{C}\hat{A}].
\end{aligned}$$

2. Aus der Definition $\hat{E}^\theta_\psi = \sum_{n=1}^d |\psi_n\rangle\langle\theta_n|$ folgt, dass $\hat{E}^\psi_\theta = \sum_{n=1}^d |\theta_n\rangle\langle\psi_n|$. Wir berechnen

$$\hat{E}^\theta_\psi\hat{E}^\psi_\theta = \sum_{n=1}^d\sum_{m=1}^d |\psi_n\rangle\langle\theta_n|\theta_m\rangle\langle\psi_m| = \sum_{n=1}^d\sum_{m=1}^d \delta_{mn}|\psi_n\rangle\langle\psi_m| = \sum_{n=1}^d |\psi_n\rangle\langle\psi_n| = \mathbb{1}$$

Damit haben wir gezeigt, dass $\hat{E}^\psi_\theta = (\hat{E}^\theta_\psi)^{-1}$. Aus der Definition erkennen wir, dass $\hat{E}^\psi_\theta = (\hat{E}^\theta_\psi)^\dagger$. Daraus folgt, dass $(\hat{E}^\psi_\theta)^\dagger = (\hat{E}^\psi_\theta)^{-1}$ und damit ist $\hat{E}^\theta_\psi$ ein *unitärer Operator*.

Schließlich zeigen wir, dass der gegebene Operator tatsächlich einen Basiswechsel herbeiführt. Dafür berechnen wir mithilfe der Orthonormalität der Basis den Erwartungswert

$$\langle\theta_j|\hat{E}^\psi_\theta\hat{A}\hat{E}^\theta_\psi|\theta_k\rangle = \sum_{n,m=1}^d \langle\theta_j|\theta_n\rangle\langle\psi_n|\hat{A}|\psi_m\rangle\langle\theta_m|\theta_k\rangle = \sum_{n,m=1}^d \delta_{jn}\langle\psi_n|\hat{A}|\psi_m\rangle\delta_{mk} = \langle\psi_j|\hat{A}|\psi_k\rangle\,.$$

3. Mithilfe des Ergebnis der letzten Aufgabe zeigen wir, dass

$$\begin{aligned}
\mathrm{tr}_\psi[\hat{A}] = \sum_{n=1}^{d} \langle\psi_n|\hat{A}|\psi_n\rangle &= \sum_{n=1}^{d} \langle\theta_n|\hat{E}^\psi_\theta \hat{A}\hat{E}^\theta_\psi|\theta_n\rangle \qquad \text{change of basis} \\
&= \mathrm{tr}_\theta[\hat{E}^\psi_\theta \hat{A}\hat{E}^\theta_\psi] \qquad \text{from definition of } \mathrm{tr}_\theta[\cdot] \\
&= \mathrm{tr}_\theta[\hat{E}^\theta_\psi \hat{E}^\psi_\theta \hat{A}] \qquad \text{using cyclic property of the trace} \\
&= \mathrm{tr}_\theta[\mathbb{1}\hat{A}] \qquad \text{operators are inverses of each other} \\
&= \mathrm{tr}_\theta[\hat{A}].
\end{aligned}$$

4. Here we start with the given commutation relation for the position and momentum operators, assume that they *can* be defined on a finite dimensional Hilbert space, and then take the trace of the commutation relation. Since we are assuming they can be defined in finite dimensions, their trace *must* also be a finite number. The result will be a contradiction, and since the trace is independent of any basis we could choose, it is therefore not possible to define $\hat{x}$ and $\hat{p}$ on a finite dimensional Hilbert space.

   So, we being by assuming that the Hilbert space is d-dimensional. Now we take the trace of $[\hat{x},\hat{p}] = i\hbar\mathbb{1}$, first the right hand side:

$$\begin{aligned}
\mathrm{tr}([\hat{x},\hat{p}]) &= \mathrm{tr}[\hat{x}\hat{p} - \hat{p}\hat{x}] \\
&= \mathrm{tr}[\hat{x}\hat{p}] - \mathrm{tr}[\hat{p}\hat{x}] \quad \text{using linearity} \\
&= \mathrm{tr}[\hat{x}\hat{p}] - \mathrm{tr}[\hat{x}\hat{p}] \quad \text{using the cyclic property} \\
&= 0.
\end{aligned}$$

   And now for the left hand side:

$$\mathrm{tr}[i\hbar\mathbb{1}] = i\hbar d \qquad \text{since } \mathbb{1} \text{ is a } d\text{-by-}d \text{ identity matrix in finite dimensions.}$$

   We therefore have $0 = i\hbar d$, which is a contradiction. The conclusion then is that it is not possible to define these operators in a finite dimensional Hilbert space.

   They can therefore only be defined in an infinite-dimensional Hilbert space; there the notion of *trace-class* operators exists, which are operators with a well-defined finite trace. A necessary (but not sufficient) condition for operators to be trace-class is that they are bounded. As it turns out $\hat{x}$ and $\hat{p}$ are not bounded operators and hence not trace-class, but that proof is more difficult.

Aufgabe 3. (? Punkte)

Lösung Aufgabe 3.

Density matrices are important objects to describe a quantum system. While a state vector $|\psi\rangle$ can only account for a quantum system in a pure state, a density matrix $\hat{\rho}$ allows us to describe quantum systems in mixed states as well.

1. Prove that the expectation value of an observable $\hat{A}$ obeys $\langle\psi|\,\hat{A}\,|\psi\rangle \geq 0$ for any $|\psi\rangle$ if and only if $\hat{A}$ has no negative eigenvalues.
   Hint: You can use the fact that the eigenbasis $\{|a_n\rangle\}$ is complete, i.e., $\sum_n |a_n\rangle\langle a_n| = \mathbf{1}$.

   Solution:
   eigenvalue of operator $\hat{A}$ in its eigenbasis: $\hat{A}\,|a_n\rangle = a_n\,|a_n\rangle$

$$\begin{aligned}
\langle\psi|\hat{A}|\psi\rangle =& \langle\psi|\mathbf{1}\hat{A}\mathbf{1}|\psi\rangle = \langle\psi|\left(\sum_n |a_n\rangle\langle a_n|\right)\hat{A}\left(\sum_m |a_m\rangle\langle a_m|\right)|\psi\rangle = \sum_{n,m}\langle\psi|a_n\rangle\langle a_n|\,\hat{A}\,|a_m\rangle\langle a_m|\psi\rangle \\
=& \sum_{n,m} a_m\langle\psi|a_n\rangle\langle a_n|a_m\rangle\langle a_m|\psi\rangle = \sum_n a_m\,|\langle a_n|\psi\rangle|^2 \geq 0 \;\text{ for }\; a_m > 0
\end{aligned}$$

2. Prove that $\hat{\rho}$ given by the expression

$$\hat{\rho} = \sum_{j=1}^{n} p_j \left|\psi_j\right\rangle \left\langle\psi_j\right| \quad . \tag{1}$$

is indeed a density matrix. Here, $p_j \in [0\,,1]$ label the probability for state $|\psi_j\rangle$. That means, show that $\hat{\rho}$ is positive semi-definite ($\langle\psi|\,\hat{\rho}\,|\psi\rangle \geq 0$ for all $|\psi\rangle$) and that $\mathrm{Tr}\,[\hat{\rho}] = 1$.

Solution:

positive semidefinite: expand general state in the basis states: $|\psi\rangle = \sum_k \alpha_k |\psi_k\rangle$

$$\langle\psi|\hat{\rho}|\psi\rangle = \sum_{j,k,l}^{n} \alpha_l^* \alpha_k p_j \langle\psi_l|\psi_j\rangle\langle\psi_j|\psi_k\rangle = \sum_{j,k,l}^{n} \alpha_l^* \alpha_k p_j \delta_{l,j}\delta_{k,j} = \sum_{j}^{n} |\alpha_j|^2 p_j \geq 0$$

trace:

$$\mathrm{Tr}(\hat{\rho}) = \sum_{k=1}^{n} \langle\psi_k|\hat{\rho}|\psi_k\rangle = \sum_{k,j=1}^{n} p_j \langle\psi_k|\,|\psi_j\rangle\langle\psi_j|\,|\psi_k\rangle = \sum_{k,j=1}^{n} p_j = 1$$

3. Consider a Hermitian operator $\hat{A}^\dagger = \hat{A}$, i.e., $\hat{A}$ is an observable. Prove for the decomposition Eq. 1 that

$$\mathrm{Tr}\left(\hat{\rho}\hat{A}\right) = \sum_{j=1}^{n} p_j \left\langle\psi_j\right|\hat{A}\left|\psi_j\right\rangle \quad , \tag{2}$$

i.e., that the expectation value of $\hat{A}$ in state $\hat{\rho}$ is the same as the expectation value with respect to p_j of the "pure state expectation values".

Solution:

$$\mathrm{Tr}(\rho A) = \sum_{k} \langle\psi_k|\hat{\rho}\hat{A}|\psi_k\rangle = \sum_{k,j} p_j \langle\psi_k|\,|\psi_j\rangle\langle\psi_j|\,\hat{A}|\psi_k\rangle = \sum_{j} p_j \langle\psi_j|\hat{A}|\psi_j\rangle$$

4. Consider the special case $n = 2$ in Eq. 1. Show that the decomposition is not unique, i.e., find pairwise different and normalized $|\psi_1\rangle\,,|\psi_2\rangle\,,|\phi_1\rangle\,,|\phi_2\rangle$ and probabilities $p_j\,,q_j \in [0\,,1]$ such that

$$\sum_{j=1}^{2} p_j \left|\psi_j\right\rangle \left\langle\psi_j\right| = \sum_{j=1}^{2} q_j \left|\phi_j\right\rangle \left\langle\phi_j\right| \quad . \tag{3}$$

Solution:

here many solutions are possible, for example we could start from

$$|\psi_1\rangle = |0\rangle\,,\; |\psi_2\rangle = |1\rangle\,, \qquad |\phi_1\rangle = \alpha_1|0\rangle + \alpha_2|1\rangle\,,\; |\phi_2\rangle = \beta_1|0\rangle + \beta_2|1\rangle\,,$$

$$\hat{\rho}_\psi = p_1 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + p_2 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} p_1 & 0 \\ 0 & 1-p_1 \end{pmatrix},$$

$$\hat{\rho}_\phi = q_1 \begin{pmatrix} |\alpha_1|^2 & \alpha_1\alpha_2^* \\ \alpha_1^*\alpha_2 & |\alpha_2|^2 \end{pmatrix} + q_2 \begin{pmatrix} |\beta_1|^2 & \beta_1\beta_2^* \\ \beta_1^*\beta_2 & |\beta_2|^2 \end{pmatrix} = \begin{pmatrix} q_1|\alpha_1|^2 + (1-q_1)|\beta_1|^2 & q_1\alpha_1\alpha_2^* + (1-q_1)\beta_1\beta_2^* \\ q_1\alpha_1^*\alpha_2 + (1-q_1)\beta_1^*\beta_2 & q_1|\alpha_2|^2 + (1-q_1)|\beta_2|^2 \end{pmatrix}$$

normalization requires $|\alpha_1|^2 + |\alpha_2|^2 = 1$ and $|\beta_1|^2 + |\beta_2|^2 = 1$, thus $\hat{\rho}_\psi = \hat{\rho}_\phi$ from the conditions for the off-diagonal elements we obtain

$$q_1 = \frac{-\beta_1\beta_2^*}{(\alpha_1\alpha_2^* - \beta_1\beta_2^*)} \qquad q_2 = \frac{\alpha_1\alpha_2^*}{(\alpha_1\alpha_2^* - \beta_1\beta_2^*)}$$

and thus

$$p_1 = \frac{\alpha_1\alpha_2^*|\beta_1|^2 - \beta_1\beta_2^*|\alpha_1|^2}{(\alpha_1\alpha_2^* - \beta_1\beta_2^*)} \qquad p_2 = \frac{\alpha_1\alpha_2^*|\beta_2|^2 - \beta_1\beta_2^*|\alpha_2|^2}{(\alpha_1\alpha_2^* - \beta_1\beta_2^*)}$$

and they have to real and positive. Defining $\beta_1\beta_2^* = |\beta_1\beta_2|e^{i\theta_\beta}$ and $\alpha_1\alpha_2^* = |\alpha_1\alpha_2|e^{i\theta_\alpha}$ we obtain

$$q_1 = \frac{|\beta_1\beta_2|}{\left(|\alpha_1\alpha_2|e^{i\bar{\theta}} + |\beta_1\beta_2|\right)} \qquad q_2 = \frac{|\alpha_1\alpha_2|e^{i\bar{\theta}}}{\left(|\alpha_1\alpha_2|e^{i\bar{\theta}} + |\beta_1\beta_2|\right)}$$
$$p_1 = \frac{|\alpha_1\alpha_2|e^{i\bar{\theta}}|\beta_1|^2 + |\beta_1\beta_2||\alpha_1|^2}{\left(|\alpha_1\alpha_2|e^{i\bar{\theta}} + |\beta_1\beta_2|\right)} \qquad p_2 = \frac{|\alpha_1\alpha_2|e^{i\bar{\theta}}|\beta_2|^2 + |\beta_1\beta_2||\alpha_2|^2}{\left(|\alpha_1\alpha_2|e^{i\bar{\theta}} + |\beta_1\beta_2|\right)}$$

with $\bar{\theta} = \theta_\alpha - \theta_\beta - \pi$ which has to be zero to have real numbers. For a simple case we can assume $|\alpha_{1,2}| \equiv 1/\sqrt{2}$ and $|\beta_1| = 1/2$, $|\beta_2| = \sqrt{3}/2$ and $\theta_\alpha = 0$ and $\theta_\beta = \pi$. E.g., we could have

$$q_1 = \frac{\sqrt{3}}{\left(2+\sqrt{3}\right)},\ q_2 = \frac{2}{\left(2+\sqrt{3}\right)} \qquad p_1 = \frac{\frac{1}{2}\left(1+\sqrt{3}\right)}{\left(2+\sqrt{3}\right)},\ p_2 = \frac{\frac{1}{2}\left(3+\sqrt{3}\right)}{\left(2+\sqrt{3}\right)}$$
$$|\psi_1\rangle = |0\rangle\,,\ |\psi_2\rangle = |1\rangle\,,\ |\phi_1\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right),\ |\phi_2\rangle = \frac{1}{2}\left(|0\rangle - \sqrt{3}\,|1\rangle\right),$$

we can test this

$$\hat{\rho}_\psi = \begin{pmatrix} p_1 & 0 \\ 0 & p_2 \end{pmatrix} = \frac{1}{2+\sqrt{3}} \begin{pmatrix} \frac{1}{2}\left(1+\sqrt{3}\right) & 0 \\ 0 & \frac{1}{2}\left(3+\sqrt{3}\right) \end{pmatrix}$$
$$\hat{\rho}_\phi = q_1 \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} + q_2 \begin{pmatrix} \frac{1}{4} & -\frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix} = \frac{1}{2+\sqrt{3}} \begin{pmatrix} \frac{1}{2}\left(\sqrt{3} + \frac{1}{2}2\right) & \sqrt{3}\frac{1}{2} - \frac{\sqrt{3}}{4}2 \\ \sqrt{3}\frac{1}{2} - \frac{\sqrt{3}}{4}2 & \frac{1}{2}\left(\sqrt{3} + \frac{3}{2}2\right) \end{pmatrix} = \hat{\rho}_\psi$$

5. A state $\hat{\rho}$ is called *pure* if there is a vector $|\psi\rangle$ such that $\hat{\rho} = |\psi\rangle\langle\psi|$. If no such a vector exists, it is called *mixed* and can be written as $\hat{\rho} = \sum_{j=1}^n p_j |\psi_j\rangle\langle\psi_j|$. Prove that $\hat{\rho}$ is a pure state if and only if $\mathrm{Tr}\left(\hat{\rho}^2\right) = 1$.
Solution:

$$\mathrm{Tr}\left(\sum_{j=1,k}^{n} p_j p_k \,|\psi_j\rangle\langle\psi_j|\,|\psi_k\rangle\langle\psi_k|\right) = \sum_j p_j^2 = 1 \text{ (if pure)},$$

and we have $\sum_j p_j = 1,\ p_j \in [0,1]$, thus only $p_j = \delta_{j,a}$ is possible for all $a \in \mathbb{N}$