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Quantum mechanics - a summary

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1 Mathematical essentials

1.1 Norm

Let E be a vector space over the field $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$. Then $\|\cdot\| : E \to [0, \infty)$ is called **norm**, if $\forall x, y \in E$, $\lambda \in \mathbb{K}$ it holds

(N1) $\|x\| \geq 0$ (**positivity**)

(N2) $\|x\| = 0 \Leftrightarrow x = 0$ (**point separating**)

(N3) $\|\lambda x\| = |\lambda| \|x\|$ (**homogeneity**)

(N4) $\|x + y\| \leq \|x\| + \|y\|$ (**triangle inequality**)

Then $(E, \|\cdot\|)$ is called **normed space**.

[1] In mathematics the scalar product usually is defined linear in the first component, contrasting the physicist definition with linearity in the second component. The reason for physicists to chose linearity in the second component is that only this way the useful Dirac notation works nicely.

1.2 Scalar product

$V \times V \ni (x,y) \mapsto \langle x|y\rangle \in \mathbb{K}$ is called **scalar product**, if $\forall x, y, y_1, y_2 \in V$ and $\alpha, \beta \in \mathbb{K}$ it holds[1]:

(i) $\langle x| \big(\alpha\, |y_1\rangle + \beta\, |y_2\rangle\big) = \alpha\, \langle x|y_1\rangle + \beta\, \langle x|y_2\rangle$

(ii) $\langle x|y\rangle = \langle y|x\rangle^*$ (**hermitian symmetry**)

(iii) $\langle x|x\rangle \geq 0$ (**positivity**)

(iv) $\langle x|x\rangle = 0 \;\Leftrightarrow\; x = 0$ (**point separating**)

(i) and (ii) together are also called **sesquilinearity**.
Every scalar product induces a norm:

$$\|\cdot\| : V \to [0,\infty)\,,\; x \mapsto \|x\| := \sqrt{\langle x|x\rangle}$$

Cauchy-Schwarz inequality:

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

1.3 Hilbert space

A Hilbert space $\big(\mathcal{H}, \langle\,\cdot\,,\,\cdot\,\rangle\big)$ is a complete normed vector space, with the norm induced by a scalar product. In the following we will simply call such a space $\mathcal{H}$ and denote vectors in it $|\psi\rangle$. If $\mathcal{H}$ is separable and $\{\big|a^{(i)}\big\rangle\}$ is an orthonormal basis (**ONB**) of $\mathcal{H}$, then $|\psi\rangle$ can be represented towards this basis as

$$|\psi\rangle \doteq \begin{pmatrix} \big\langle a^{(1)}\big|\psi\big\rangle \\ \big\langle a^{(2)}\big|\psi\big\rangle \\ \vdots \end{pmatrix}.$$

An element $\langle\psi|$ of the dual space can then be represented as

$$\begin{aligned}\langle\psi| &\doteq \big(\langle\psi|a^{(1)}\rangle\,,\; \langle\psi|a^{(2)}\rangle\,,\; \ldots\big) \\ &= \big(\langle a^{(1)}|\psi\rangle^*\,,\; \langle a^{(2)}|\psi\rangle^*\,,\; \ldots\big)\,.\end{aligned}$$

When not stated differently, we will always assume $|\psi\rangle$ to be normed to one, i.e. $\langle\psi|\psi\rangle = 1$.

1.4 Operators

Let $\mathcal{H}$ be a Hilbert space, then a linear map

$$\hat{A} : \mathcal{H} \to \mathcal{H}\,,\; |\psi\rangle \mapsto \hat{A}\,|\psi\rangle$$

is called **operator**. If $\mathcal{H}$ is separable and $\{\big|a^{(i)}\big\rangle\}$ is an ONB of $\mathcal{H}$, we can give the matrix representation of $\hat{A}$ towards this basis as

$$\hat{A} \doteq \begin{pmatrix} \big\langle a^{(1)}\big|\,\hat{A}\,\big|a^{(1)}\big\rangle & \big\langle a^{(1)}\big|\,\hat{A}\,\big|a^{(2)}\big\rangle & \ldots \\ \big\langle a^{(2)}\big|\,\hat{A}\,\big|a^{(1)}\big\rangle & \big\langle a^{(2)}\big|\,\hat{A}\,\big|a^{(2)}\big\rangle & \ldots \\ \vdots & \vdots & \ddots \end{pmatrix}.$$

The set of all linear continuous operators on $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$.

1.5 Test for equality of operators

Proposition 1 (Test for equality of operators).
Let $\mathcal{H}$ be a complex Hilbert space and $\hat{A}, \hat{B}$ two linear (not necessarily continuous) operators on $\mathcal{H}$ with the same domain $\mathcal{D} := \mathrm{dom}(\hat{A}) = \mathrm{dom}(\hat{B})$ and with $\mathrm{im}(\hat{A}), \mathrm{im}(\hat{B}) \subseteq \mathcal{D}$. Then

$$\forall x \in \mathcal{D} \;:\; \langle x, \hat{A}x\rangle = \langle x, \hat{B}x\rangle \quad\Leftrightarrow\quad \hat{A} = \hat{B}\,.$$

Proposition 2 (Simpler version for continuous operators).
Let $\mathcal{H}$ be a complex Hilbert space and $\hat{A}, \hat{B} \in \mathcal{B}(\mathcal{H})$. Then

$$\forall x \in \mathcal{H} \;:\; \langle x|\,\hat{A}\,|x\rangle = \langle x|\,\hat{B}\,|x\rangle \quad\Leftrightarrow\quad \hat{A} = \hat{B}\,.$$

1.6 Basis change

Let there be two ONBs $\{\big|a^{(i)}\big\rangle\}$ and $\{\big|a^{(i)}\big\rangle\}$. Then there exists a unitary transformation $\hat{U}$ that transforms from one to the other basis, i.e.

$$\hat{U} = \sum_i |b^{(i)}\rangle\langle a^{(i)}|\,.$$

1.7 Adjoint operator

Let $\mathcal{H}$ be a Hilbert space and $\hat{A} : \mathcal{H} \to \mathcal{H}$ an operator on $\mathcal{H}$. Then there exists exactly one $\hat{A}^\dagger : \mathcal{H} \to \mathcal{H}$, such that $\forall \psi, \phi \in \mathcal{H}$:

$$\langle\hat{A}\psi|\phi\rangle = \langle\psi|\hat{A}^\dagger\phi\rangle\,.$$

$\hat{A}^\dagger$ is called the adjoint of $\hat{A}$. The adjoint operation conforms with

$$\begin{aligned}\big(\lambda\hat{A}\big)^\dagger &= \lambda^*\hat{A}^\dagger\,, \\ \big(\hat{A}^\dagger\big)^\dagger &= \hat{A}\,, \\ \big(\hat{A}+\hat{B}\big)^\dagger &= \hat{A}^\dagger + \hat{B}^\dagger\,, \\ \big(\hat{A}\hat{B}\big)^\dagger &= \hat{B}^\dagger\hat{A}^\dagger\,.\end{aligned}$$

Decomposition

Let $\hat{A}$ be an arbitrary operator, then we define the hermitian components as

$$\hat{A}_h \coloneqq \frac{1}{2}\big(\hat{A}+\hat{A}^\dagger\big)\,, \qquad \text{mit} \;\; \hat{A}_h^\dagger = \hat{A}_h$$

and the anti-hermitian component as

$$\hat{A}_a \coloneqq \frac{1}{2}\big(\hat{A}-\hat{A}^\dagger\big)\,, \qquad \text{mit} \;\; \hat{A}_a^\dagger = -\hat{A}_a$$

Obviously $\hat{A} = \hat{A}_h + \hat{A}_a$.

Dyadic product:

$$\big(\left|\psi\right\rangle\left\langle\phi\right|\big)^\dagger = \left|\phi\right\rangle\left\langle\psi\right| \,.$$

Cauchy-Schwarz inequality:

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

1.8 Trace

Let $\{\left|n_i\right\rangle \;:\; i\in\mathbb{N}\}$ be an arbitrary ONB. The trace of an operator $\hat{A}:\mathcal{H}\to\mathcal{H}$ is defined as

$$\operatorname{Tr}\hat{A} \coloneqq \sum_i \left\langle n_i\right|\hat{A}\left|n_i\right\rangle \,.$$

It is independent of the chosen ONB. For dyadic products one finds

$$\operatorname{Tr}\big(\left|\psi\right\rangle\left\langle\phi\right|\big) = \left\langle\phi|\psi\right\rangle \,.$$

The trace arguments can be cyclic permuted:

$$\operatorname{Tr}\big(\hat{A}\hat{B}\hat{C}\big) = \operatorname{Tr}\big(\hat{B}\hat{C}\hat{A}\big) = \operatorname{Tr}\big(\hat{C}\hat{A}\hat{B}\big)\,.$$

For a unitary operator $\hat{U}$, i.e. $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \mathbb{1}$, we find

$$\operatorname{Tr}\big(\hat{U}^\dagger\hat{A}\hat{U}\big) = \operatorname{Tr}\hat{A}\,.$$

1.9 Unitary diagonalization of normal matrices

Let $A\in\mathbb{C}^{n\times n}$ be a normal matrix, i.e. $A^\dagger A = AA^\dagger$, with eigenvalues $\{\lambda_1,\ldots,\lambda_n\}$ and eigenvectors $\{v_1,\ldots,v_n\}$. Then

$$A = U\operatorname{diag}(\lambda_1,\ldots,\lambda_n)U^\dagger\,.$$

with the unitary matrix

$$U \coloneqq (v_1\ldots v_n)\,.$$

Particularly hermitian matrices ($A^\dagger = A$) can be diagonalized this way, which is of importance for observables in quantum mechanics.

1.10 Simultaneous diagonalization

Eigenvectors of different eigenvalues ore orthogonal.
Let $\mathcal{H}$ be a Hilbert space and $\hat{A},\hat{B}\in\mathcal{B}(\mathcal{H})$ with $[\hat{A},\hat{B}]=0$. Then $\hat{A}$ and $\hat{B}$ are simultaneously diagonalizable, i.e. there exists an ONB $\{\left|a_i,b_i\right\rangle\}$ with

$$\begin{aligned}\hat{A}\left|a_i,b_i\right\rangle &= a_i\left|a_i,b_i\right\rangle\,,\\ \hat{B}\left|a_i,b_i\right\rangle &= b_i\left|a_i,b_i\right\rangle\,,\\ \left\langle a_i,b_i|a_j,b_j\right\rangle &= \delta_{i,j}\,.\end{aligned}$$

1.11 Functional calculus for normal matrices

Let $A\in\mathbb{C}^{n\times n}$ be a normal matrix and $f:\sigma(A)\to\mathbb{C}$ a function defined on the spectrum of A. We then define

$$f(A)\coloneqq U\operatorname{diag}\big(f(\lambda_1),\ldots,f(\lambda_n)\big)U^\dagger$$

and find

$$\begin{aligned}\big(\alpha f+\beta g\big)(A) &= \alpha f(A)+\beta g(A)\\ \big(f\cdot g\big)(A) &= f(A)g(A)\\ \overline{f}(A) &= \big(f(A)\big)^*\,.\end{aligned}$$

Also $f(A)$ is normal and for $g:\sigma(f(A))\to\mathbb{C}$ we find

$$\big(g\circ f\big)(A) = g(f(A))\,.$$

For a further arbitrary unitary matrix V we furthermore find

$$Vf(A)V^\dagger = f(VAV^\dagger)\,.$$

1.12 Spectrum of an operator

Let $\mathcal{H}$ be a Hilbert space and $A:\mathcal{H}\to\mathcal{H}$ a continuous linear operator on $\mathcal{H}$. Then the spectrum of T is defined as

$$\sigma(A)\coloneqq\big\{\lambda\in\mathbb{C}:(A-\lambda\mathbb{1})\text{ not}\\ \text{continuously invertible in }\mathcal{H}\big\}\,.$$

1.13 Spectral decomposition

Let $\hat{A} \in \mathcal{B}(\mathcal{H})$ be normal with orthonormal eigenbasis $\{|a_i\rangle\}$. Then $\hat{A}$ can be written in spectral decomposition

$$\hat{A} = \sum_i a_i |a_i\rangle \langle a_i| \ .$$

and for $f : \sigma(\hat{A}) \to \mathbb{C}$ we find

$$f(\hat{A}) = \sum_i f(a_i) |a_i\rangle \langle a_i| \ .$$

For example we find

$$\begin{aligned}
e^{\alpha\hat{A}} &= \sum_{n=0}^{\infty} e^{\alpha a_i} |a_i\rangle \langle a_i| \\
e^{\alpha\hat{A}} e^{-\alpha\hat{A}} &= \sum_{i=0}^{\infty} e^{\alpha a_i} |a_i\rangle \langle a_i| \sum_{j=0}^{\infty} e^{-\alpha a_j} |a_j\rangle \langle a_j| \\
&= \sum_{i=0}^{\infty} |a_i\rangle \langle a_i| = \mathbb{1} \\
\frac{\mathrm{d}}{\mathrm{d}\alpha} e^{\alpha\hat{A}} &= \frac{\mathrm{d}}{\mathrm{d}\alpha} \sum_{i=0}^{\infty} e^{\alpha a_i} |a_i\rangle \langle a_i| = \sum_{i=0}^{\infty} e^{\alpha a_i} a_i |a_i\rangle \langle a_i| \\
&= \sum_{i=0}^{\infty} e^{\alpha a_i} \hat{A} |a_i\rangle \langle a_i| = \hat{A} e^{\alpha\hat{A}} .
\end{aligned}$$

1.14 Commutator and anti-commutator

Commutator:

$$[A, B] \coloneqq AB - BA$$

Anti-commutator:

$$\{A, B\} \coloneqq AB + BA \tag{1.1}$$

Relations:

$$\begin{aligned}
[A, A] &= 0 \\
[A, B] &= -[B, A] \\
[A + B, C] &= [A, C] + [B, C] \\
[AB, C] &= A[B, C] + [A, C]B \\
[A, BC] &= B[A, C] + [A, B]C \\
0 &= [A, [B, C]] + [B, [C, A]] + [C, [A, B]]
\end{aligned}$$

1.15 Baker-Campbell-Hausdorff-Relation

For $\hat{A}, \hat{B} \in \mathcal{B}(\mathcal{H})$ one finds

$$e^{\lambda\hat{A}} \hat{B} e^{-\lambda\hat{A}} = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} [\hat{A}, \hat{B}]_{(k)}$$

with

$$[\hat{A}, \hat{B}]_{(0)} = \hat{B} \qquad [\hat{A}, \hat{B}]_{(k)} = [\hat{A}, [\hat{A}, \hat{B}]_{(k-1)}] \, .$$

If $[\hat{A}, [\hat{A}, \hat{B}]] = 0 = [\hat{B}, [\hat{A}, \hat{B}]]$, it holds the **Baker-Campbell-Hausdorff-Relation**

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A}+\hat{B}} e^{\frac{1}{2}[\hat{A},\hat{B}]} \, .$$

1.16 Continuous Bases

Since we expect the momentum operator $\hat{\boldsymbol{p}}$ to have arbitrary eigenvalues $\boldsymbol{p} \in \mathbb{R}^3$, we must consider so called continuous bases. They fulfill

$$\begin{aligned}
\mathbb{1} &= \int \mathrm{d}\xi \ |\xi\rangle \langle\xi| \ , \\
|\alpha\rangle &= \int \mathrm{d}\xi \ |\xi\rangle \langle\xi|\alpha\rangle \ .
\end{aligned}$$

1.17 Fourier transformation

$$\begin{aligned}
\langle \boldsymbol{x}|\psi\rangle = \psi(\boldsymbol{x}) &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}} \mathrm{d}^3k \, e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \tilde{\psi}(\boldsymbol{k}) \, , \\
\langle \boldsymbol{k}|\psi\rangle = \tilde{\psi}(\boldsymbol{k}) &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}} \mathrm{d}^3x \, e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \psi(\boldsymbol{x}) \, .
\end{aligned}$$

Using $\boldsymbol{p} = \hbar\boldsymbol{k}$ as the momentum space basis, one has

$$\begin{aligned}
\langle \boldsymbol{x}|\psi\rangle = \psi(\boldsymbol{x}) &= \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}} \mathrm{d}^3p \, e^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}} \tilde{\psi}(\boldsymbol{p}) \, , \\
\langle \boldsymbol{p}|\psi\rangle = \tilde{\psi}(\boldsymbol{p}) &= \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}} \mathrm{d}^3x \, e^{-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}} \psi(\boldsymbol{x}) \, .
\end{aligned}$$

2 Physical principles

2.1 Momentum operator in position basis

One finds

$$\langle \boldsymbol{x}| \, \hat{\boldsymbol{p}} \, |a\rangle = -i\hbar \, \boldsymbol{\nabla}_{\boldsymbol{x}} \langle \boldsymbol{x}|a\rangle = -i\hbar \, \boldsymbol{\nabla}_{\boldsymbol{x}} \psi_a(\boldsymbol{x}) \, .$$

Proof for 1D: In momentum space we find

$$\begin{aligned}
\langle x| \, \hat{p} \, |a\rangle &= \int \mathrm{d}p \, \langle x|p\rangle \langle p| \, \hat{p} \, |a\rangle \\
&= \int \mathrm{d}p \, \langle x|p\rangle \, p\tilde{\psi}_a(p) \\
&= \int \mathrm{d}p \mathcal{N} e^{\frac{i}{\hbar}px} p\tilde{\psi}_a(p) \\
&= \mathcal{N} \int \mathrm{d}p \, \big(-i\hbar \, \partial_x e^{\frac{i}{\hbar}px} \big) \tilde{\psi}_a(p) \\
&= -i\hbar \, \partial_x \mathcal{N} \int \mathrm{d}p \, e^{\frac{i}{\hbar}px} \tilde{\psi}_a(p) \\
&= -i\hbar \, \partial_x \psi_a(x) \, ,
\end{aligned}$$

where $\mathcal{N} = (2\pi\hbar)^{-1/2}$.

2.2 Position operator in momentum basis

In analogy to the above situation one finds

$$\langle \boldsymbol{p}| \hat{\boldsymbol{x}} |a\rangle = i\hbar \boldsymbol{\nabla}_{\boldsymbol{p}} \tilde{\psi}_a(\boldsymbol{p}) \,.$$

2.2.1 Eigenstates of the momentum operator in 1D

We are now looking for states that fulfill

$$p \langle x|p\rangle = \langle x| \hat{p} |p\rangle = -i\hbar\partial_x \langle x|p\rangle \ .$$

This ordinary differential equation of first order is solved by

$$\langle x|p\rangle = \mathcal{N} e^{\frac{i}{\hbar}px} \,, \tag{2.1}$$

with the normalization constant still to be derived. Using

$$\begin{aligned}
\delta(x'-x'') = \langle x'|x''\rangle &= \int \mathrm{d}p \, \langle x'|p\rangle \langle p|x''\rangle \\
&= |\mathcal{N}|^2 \int \mathrm{d}p \, e^{\frac{i}{\hbar}p(x'-x'')} \\
&= 2\pi\hbar|\mathcal{N}|^2 \\
\Rightarrow \quad \mathcal{N} &= \frac{1}{\sqrt{2\pi\hbar}} \,.
\end{aligned}$$

This finally leads to transformation rules between the position and the momentum description, i.e.

$$\begin{aligned}
\tilde{\psi}_a(p) &= \frac{1}{(2\pi\hbar)^{1/2}} \int \mathrm{d}p \, e^{-\frac{i}{\hbar}px} \psi_a(x) \,, \\
\psi_a(x) &= \frac{1}{(2\pi\hbar)^{1/2}} \int \mathrm{d}p \, e^{\frac{i}{\hbar}px} \tilde{\psi}_a(p) \,,
\end{aligned}$$

which obviously is a Fourier transformation.

2.3 Derivation of the canonical commutation relation

From classical mechanics we know that momentum is the generator for translations. Let us try to transfer this concept to quantum mechanics.

The translation operator

We implicitly define the translation operator by its action

$$\hat{T}(a) |x\rangle = |x+a\rangle \ .$$

on a position state, i.e. it »shifts« the state to the right by the real valued distance a. Using another position ket $|y\rangle$ we find

$$\begin{aligned}
\langle y| \hat{T}(a)^\dagger |x\rangle = \langle x| \hat{T}(a) |y\rangle^* &= \langle x|y+a\rangle^* \\
&= \langle y+a|x\rangle = \delta((y+a)-x) \\
&= \delta(y-(x-a)) = \langle y|x-a\rangle \ .
\end{aligned}$$

Since this relation holds for all $\langle y|$ we have

$$\hat{T}(a)^\dagger |x\rangle = |x-a\rangle$$

and see that

$$\hat{T}(a)^\dagger \hat{T}(a) = \mathbb{1} = \hat{T}(a)\hat{T}(a)^\dagger \,,$$

i.e. the translation operator $\hat{T}(a)$ is a unitary operator. Furthermore, it is reasonable to demand

$$\lim_{a\to 0} \hat{T}(a) = \mathbb{1} \quad \text{and} \quad \hat{T}(a)\hat{T}(b) = \hat{T}(a+b) \,.$$

This already suffices for using the Stone theorem (see appendix) which guarantees the unique existence of a hermitian operator $\hat{G}$, called the **generator** of the transformation/unitary operator, for which holds

$$\hat{T}(a) = e^{-i\hat{G}a} \,.$$

Since we know from classical mechanics that momentum is the generator for translations we can try using the momentum operator, i.e. $\hat{G} = \hat{p}/\hbar$, where we divided by $\hbar$ to get the units correct. Indeed we find

$$\begin{aligned}
\hat{T}(a) |x\rangle = \hat{T}(a) &\int \mathrm{d}p \, |p\rangle \langle p|x\rangle \\
&= \int \mathrm{d}p \, e^{-\frac{i}{\hbar}\hat{p}a} |p\rangle \langle p|x\rangle \\
&= \int \mathrm{d}p \, e^{-\frac{i}{\hbar}pa} |p\rangle \langle p|x\rangle
\end{aligned}$$

and using (2.1) we obtain

$$\begin{aligned}
\hat{T}(a) |x\rangle &= \int \mathrm{d}p \, \mathcal{N} e^{-\frac{i}{\hbar}p(x+a)} |p\rangle \\
&= \int \mathrm{d}p \, \langle p|x+a\rangle |p\rangle \\
&= \int \mathrm{d}p \, |p\rangle \langle p|x+a\rangle \\
&= |x+a\rangle \ .
\end{aligned}$$

In analogy one finds in 3D that

The canonical commutator relation

We will now consider a state $|\psi_x\rangle$ that is well concentrated around x. The translated state $\hat{T}(a)\,|\psi\rangle$ will be denoted by $|\psi_{x+a}\rangle$. Then

$$\hat{x}\hat{T}(\mathrm{d}a)\,|\psi_x\rangle = \hat{x}\,|\psi_{x+\mathrm{d}a}\rangle \approx (x+\mathrm{d}a)\,|\psi_{x+\mathrm{d}a}\rangle$$

and

$$\hat{T}(\mathrm{d}a)\hat{x}\,|\psi_x\rangle \approx x\hat{T}(\mathrm{d}a)\,|\psi_x\rangle = x\,|\psi_{x+\mathrm{d}a}\rangle$$

Combining both results yields

$$\begin{aligned}[\hat{x},\hat{T}(\mathrm{d}a)]\,|\psi_x\rangle &= \hat{x}\hat{T}(\mathrm{d}a)\,|\psi_x\rangle - \hat{T}(\mathrm{d}a)\hat{x}\,|\psi_x\rangle \\ &\approx \mathrm{d}a\,|\psi_{x+\mathrm{d}a}\rangle \\ &\approx \mathrm{d}a\,|\psi_x\rangle\ ,\end{aligned}$$

and hence

$$[\hat{x},\hat{T}(\mathrm{d}a)] \approx \mathrm{d}a\mathbb{1}\,. \tag{2.2}$$

Furthermore, for small translations we can break the series expansion of $\hat{T}(a)$ after the linear term, i.e.

$$\hat{T}(\mathrm{d}a) = e^{-\frac{i}{\hbar}\hat{p}\,\mathrm{d}a} \approx \mathbb{1} - \frac{i}{\hbar}\hat{p}\,\mathrm{d}a\,,$$

and find

$$[\hat{x},\hat{T}(\mathrm{d}a)] \approx [\hat{x},\mathbb{1} - \frac{i}{\hbar}\hat{p}\,\mathrm{d}a] = [\hat{x},-\frac{i}{\hbar}\hat{p}\,\mathrm{d}a]$$

Combining this with (2.2) we finally find

$$\begin{aligned}&[\hat{x},-\frac{i}{\hbar}\hat{p}\,\mathrm{d}a] = \mathrm{d}a\mathbb{1} \\ \Rightarrow\ &[\hat{x},\hat{p}] = i\hbar\,\mathbb{1}\,.\end{aligned}$$

2.4 Further implications of the fundamental commutator relation

From $[\hat{\boldsymbol{x}},\hat{\boldsymbol{p}}] = i\hbar$ we can derive

$$\begin{aligned}[\hat{\boldsymbol{x}}^n,\hat{\boldsymbol{p}}] &= n\,i\hbar\,\hat{\boldsymbol{x}}^{n-1} \\ [\hat{\boldsymbol{x}},\hat{\boldsymbol{p}}^n] &= n\,i\hbar\,\hat{\boldsymbol{p}}^{n-1}\,.\end{aligned}$$

When $V(\hat{\boldsymbol{x}})$ and $V(\hat{\boldsymbol{p}})$ are series expandable, one finds

$$\begin{aligned}[V(\hat{\boldsymbol{x}}),\hat{\boldsymbol{p}}] &= i\hbar\,V'(\hat{\boldsymbol{x}}) \\ [\hat{\boldsymbol{x}},V(\hat{\boldsymbol{p}})] &= i\hbar\,V'(\hat{\boldsymbol{p}})\,.\end{aligned}$$

2.5 Transformations and Generators

An **infinitesimal transformation** is (to first order) given by

$$A(\mathrm{d}\varepsilon) = \mathbb{1} - iG\,\mathrm{d}\varepsilon\,,$$

where G is called **generator** of the transformation. Finite transformation with the variable parameter ε can then vividly be constructed as

$$A(\varepsilon) = \lim_{n\to\infty}\Big(\mathbb{1} - iG\,\frac{\varepsilon}{n}\Big)^n = e^{-iG\varepsilon}\,.$$

Starting with the infinitesimal translation

$$\hat{T}(\mathrm{d}\boldsymbol{x}) = \mathbb{1} - \frac{i}{\hbar}\hat{\boldsymbol{p}}\cdot\mathrm{d}\boldsymbol{x}$$

one obtains the translation

$$\hat{T}(\boldsymbol{x}) = e^{-\frac{i}{\hbar}\hat{\boldsymbol{p}}\cdot\boldsymbol{x}}\,.$$

Starting with the infinitesimal rotation

$$\hat{D}(\boldsymbol{n},\mathrm{d}\phi) = \mathbb{1} - \frac{i}{\hbar}\big(\hat{\boldsymbol{J}}\cdot\boldsymbol{n}\big)\,\mathrm{d}\phi$$

yields the rotation

$$\hat{D}(\boldsymbol{n},\phi) = e^{-\frac{i}{\hbar}\hat{\boldsymbol{J}}\cdot\boldsymbol{n}\,\phi}\,,$$

where $\boldsymbol{n}$ denotes a unit vector on the rotation axis.

transformation	G	ε
translation	$\hat{\boldsymbol{p}}/\hbar$	$\boldsymbol{x}$
rotation	$\hat{\boldsymbol{J}}/\hbar$	$\boldsymbol{n}\,\phi$
time evolution	$\hat{H}/\hbar$	t

Table 1: Generators in quantum mechanics.

2.6 Angular momentum and spin

The rotational group of the usual three-dimensional space is governed by non-vanishing commutators of the rotation matrices D_x, D_y and D_z. Demanding the same commutator relations for the generators of rotations on a Hilbert space, one obtains the fundamental commutator relation of angular momentum and spin, i.e.

$$[\hat{J}_i,\hat{J}_j] = i\hbar\,\varepsilon_{ijk}\hat{J}_k\,,$$

The lowest-dimensional realization of this commutator algebra is found in a 2-dimensional Hilbert space $\mathcal{H}\simeq\mathbb{C}^2$. In nature it is realized by so called spin-1/2 systems. The spin operators, in the spin-1/2 case denoted by $\hat{S}_i$ instead of $\hat{J}_i$ are given by

$$\hat{S}_i = \frac{\hbar}{2}\hat{\sigma}_i\,,\qquad \hat{\boldsymbol{S}} = (\hat{S}_1,\hat{S}_2,\hat{S}_3)^{\mathsf{T}}$$

with the Pauli operators

$$\begin{aligned}\hat{\sigma}_1 &\coloneqq |+\rangle\langle-| + |-\rangle\langle+| \\ \hat{\sigma}_2 &\coloneqq -i\,|+\rangle\langle-| + i\,|-\rangle\langle+| \\ \hat{\sigma}_3 &\coloneqq |+\rangle\langle+| - |-\rangle\langle-|\,.\end{aligned}$$

The states $|+\rangle$ and $|-\rangle$ denote the eigenstates of $\hat{\sigma}_3$ with eigenvalues $+1$ and -1. In the canonical basis

$$\{\,|+\rangle \doteq \left(\begin{smallmatrix}1\\0\end{smallmatrix}\right),\ |-\rangle \doteq \left(\begin{smallmatrix}0\\1\end{smallmatrix}\right)\}$$

they take the form

$$\hat{\sigma}_1 \doteq \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \quad \hat{\sigma}_2 \doteq \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \quad \hat{\sigma}_3 \doteq \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

and are called **Pauli matrices**.
They fulfill

$$\begin{aligned}\{\hat{\sigma}_k, \hat{\sigma}_\ell\} &= 2\delta_{k\ell}\,, \\ [\hat{\sigma}_k, \hat{\sigma}_\ell] &= 2i\,\varepsilon_{k\ell m}\hat{\sigma}_m\,.\end{aligned}$$

In general $|S_i;\pm\rangle$ is the eigenstate of $\hat{S}_i$ with eigenvalues $\pm\hbar/2$. We then have

$$\begin{aligned}|S_3;+\rangle &= |+\rangle \doteq \begin{pmatrix}1\\0\end{pmatrix} \\ |S_3;-\rangle &= |-\rangle \doteq \begin{pmatrix}0\\1\end{pmatrix}\,.\end{aligned}$$

and find

$$\begin{aligned}|S_1;+\rangle &= \frac{1}{\sqrt{2}}\big(\,|+\rangle + |-\rangle\,\big) \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \\ |S_1;-\rangle &= \frac{1}{\sqrt{2}}\big(\,|+\rangle - |-\rangle\,\big) \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}, \\ |S_2;+\rangle &= \frac{1}{\sqrt{2}}\big(\,|+\rangle + i\,|-\rangle\,\big) \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}, \\ |S_2;+\rangle &= \frac{1}{\sqrt{2}}\big(\,|+\rangle - i\,|-\rangle\,\big) \doteq \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix},\end{aligned}$$

while for each of these states one has the choice of choosing a different arbitrary phase.
Spin-1/2 operators in an arbitrary direction can be written as

$$\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n}\,.$$

For a rotation along $\boldsymbol{n}$ with angle ϕ one finds

$$\begin{aligned}\hat{D}(\boldsymbol{n},\phi) &= e^{-\frac{i}{\hbar}\hat{\boldsymbol{S}}\cdot\boldsymbol{n}\phi} \\ &= \mathbb{1}\cos(\phi/2) - i\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n}\sin(\phi/2)\,.\end{aligned}$$

2.6.1 Spin precession

Let's consider the case of an arbitrary spin-1/2-state $|\alpha\rangle$ that gets rotated around the z-axis by the angle ϕ, i.e. the rotated state is

$$|\alpha\rangle \to |\alpha\rangle_R = \hat{D}_z(\phi)\,|\alpha\rangle\,.$$

We now want to obtain the expectation value of the spin z-component, i.e.

$$\left\langle \hat{S}_x \right\rangle_{\alpha_R} = \langle\alpha|\,\hat{D}_z^\dagger(\phi)\hat{S}_x\hat{D}_z(\phi)\,|\alpha\rangle\,.$$

We find

$$\begin{aligned}\hat{D}_z^\dagger(\phi)\hat{S}_x\hat{D}_z(\phi) &= e^{\frac{i}{\hbar}\hat{S}_z\phi}\hat{S}_x e^{-\frac{i}{\hbar}\hat{S}_z\phi} \\ &\overset{\text{BCH}}{=} \hat{S}_x\cos\phi - \hat{S}_y\sin\phi\,,\end{aligned}$$

which holds for all angular momentum operator algebras. Finally, we have

$$\left\langle \hat{S}_x \right\rangle_{\alpha_R} = \left\langle \hat{S}_x \right\rangle_{\alpha}\cos\phi - \left\langle \hat{S}_y \right\rangle_{\alpha}\sin\phi\,,$$

which is a very intuitive result.
Less intuitive is the fact, that a rotation by 2π maps $|\alpha\rangle \to -\,|\alpha\rangle$, i.e. a 4π rotation is needed to get back to the original state.
For an arbitrary direction $\boldsymbol{n}$ of the spin measurement apparatus we find the positive eigenvalue state

$$|\boldsymbol{S}\cdot\boldsymbol{n};+\rangle = e^{-i\alpha/2}\cos\frac{\beta}{2}\,|+\rangle + e^{i\alpha/2}\sin\frac{\beta}{2}\,|-\rangle\,.$$

2.6.2 Subsequent spin measurements

Let $\boldsymbol{a},\boldsymbol{b}\in\mathbb{R}^3$. Then

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{a})(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{b}) = \boldsymbol{a}\cdot\boldsymbol{b} + i\hat{\boldsymbol{\sigma}}\cdot(\boldsymbol{a}\times\boldsymbol{b})\,.$$

2.7 Uncertainty

The expectation value of an observable (hermitian operator) $\hat{A}$ in the state $|\psi\rangle$ is defined as

$$\langle\hat{A}\rangle_\psi \coloneqq \langle\psi|\,\hat{A}\,|\psi\rangle\,.$$

The variance of an observable (a hermitian operator) $\hat{A}$ in the state $|\psi\rangle$ is defined as

$$\begin{aligned}\mathrm{Var}(\hat{A}) &\coloneqq \langle\psi|\,\big(\hat{A} - \langle\hat{A}\rangle_\psi\big)^2\,|\psi\rangle \\ &= \langle\hat{A}^2\rangle_\psi - \langle\hat{A}\rangle_\psi^2\,,\end{aligned}$$

and the standard deviation as

$$\Delta A := \sqrt{\mathrm{Var}(\hat{A})} = \sqrt{\langle\psi|\left(\hat{A} - \langle\hat{A}\rangle_\psi\right)^2|\psi\rangle}\,.$$

For two observables $\hat{A}$, $\hat{B}$ one has

$$\Delta A\,\Delta B \geq \frac{1}{2}\Big|\langle\psi|\,[\hat{A},\hat{B}]\,|\psi\rangle\Big|\,.$$

Immediately it follows the **Heisenberg uncertainty relation**

$$\Delta x\,\Delta p \geq \frac{\hbar}{2}\,.$$

2.8 Schrödinger equation and time evolution

The time evolution is determined by the partial differential equation

$$i\hbar\frac{\partial}{\partial t}|\psi,t\rangle = \hat{H}|\psi,t\rangle\ ,$$

called **time dependent Schrödinger equation**. Integration yields

$$|\psi,t\rangle = \hat{U}(t)|\psi\rangle$$

with the **time evolution operator**

$$\hat{U}(t) := e^{-\frac{i}{\hbar}\hat{H}t}$$

and $|\psi\rangle = |\psi,0\rangle$ is the sate at time $t=0$. Solving the **time-independent Schrödinger equation**

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

yields the energy eigenstates of the Hamiltonian. Expectation values evolve as

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle_\psi(t) = \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi,t|\hat{A}|\psi,t\rangle = \langle\psi,t|\frac{i}{\hbar}[\hat{H},\hat{A}]|\psi,t\rangle\ .$$

2.9 Continuity equation for probability density

$$\frac{\partial\rho(\boldsymbol{x},t)}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{j}(\boldsymbol{x},t) = 0\,,$$

with the **probability density**

$$\rho(\boldsymbol{x},t) = |\psi(\boldsymbol{x},t)|^2$$

and the **probability current density**

$$\boldsymbol{j}(\boldsymbol{x},t) = -\frac{i\hbar}{2m}\Big(\psi^*(\boldsymbol{x},t)\boldsymbol{\nabla}\psi(\boldsymbol{x},t) - \psi(\boldsymbol{x},t)\boldsymbol{\nabla}\psi^*(\boldsymbol{x},t)\Big)\,.$$

2.10 Pictures of quantum mechanics

In the Schrödinger picture the time dependence is encoded in the states, while observables remain time-independent.
In the Heisenberg picture all time dependence is stripped to the operators, and the states remain time-independent.
The Dirac picture is a mixture between both previous pictures. Let's say the Hamiltonian is given by $\hat{H} = \hat{H}_0 + \hat{H}_1$, where we call $\hat{H}_0$ the trivial part of the Hamiltonian. Then we set

$$\hat{U}_0(t) := e^{-\frac{i}{\hbar}\hat{H}_0 t}\,.$$

The resulting time-dependence can be seen in table 2.

picture	Hamiltonian	operator	state
Schrödinger	$\hat{H}$	$\hat{A}$	$\lvert\psi,t\rangle = \hat{U}(t)\lvert\psi\rangle$
Heisenberg	$\hat{H}_H = \hat{H}$	$\hat{A}_H = \hat{U}^\dagger(t)\hat{A}\hat{U}(t)$	$\lvert\psi\rangle_H = \lvert\psi\rangle$
Dirac / interaction	$\hat{H}_D = \hat{H}$	$\hat{A}_D = \hat{U}_0^\dagger(t)\hat{A}\hat{U}_0(t)$	$\lvert\psi,t\rangle_D = \hat{U}_0^\dagger(t)\hat{U}(t)\lvert\psi\rangle$

Table 2: Pictures of quantum mechanics.

2.11 Time evolution in Heisenberg picture

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{A}_H(t) = \frac{i}{\hbar}[\hat{H},\hat{A}_H(t)]$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle_\psi(t) = \langle\psi|\frac{i}{\hbar}[\hat{H},\hat{A}_H(t)]|\psi\rangle$$

2.12 Ehrenfest theorem

For the Hamiltonian

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{x}})$$

we find

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \psi, t | \hat{\boldsymbol{x}} | \psi, t \rangle = \frac{1}{m} \langle \psi, t | \hat{\boldsymbol{p}} | \psi, t \rangle \,,$$
$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \psi, t | \hat{\boldsymbol{p}} | \psi, t \rangle = - \langle \psi, t | \boldsymbol{\nabla} V(\hat{\boldsymbol{x}}) | \psi, t \rangle \,.$$

2.13 Gaussian wave packet

Gaussian wave packet with standard deviation a:

$$\langle \boldsymbol{x} | \psi \rangle = \psi(\boldsymbol{x}) = \left(\frac{1}{2\pi a^2} \right)^{3/4} e^{-\boldsymbol{x}^2/4a^2}$$
$$\langle \boldsymbol{k} | \psi \rangle = \tilde{\psi}(\boldsymbol{k}) = \left(\frac{2a^2}{\pi} \right)^{3/4} e^{-a^2 \boldsymbol{k}^2}$$
$$\langle \psi | \hat{x} | \psi \rangle = 0$$
$$\langle \psi | \hat{x}^2 | \psi \rangle = a^2$$
$$\langle \psi | \hat{p}_x | \psi \rangle = 0$$
$$\langle \psi | \hat{p}_x^2 | \psi \rangle = \hbar^2/4a^2$$
$$\Delta x \, \Delta p_x = \hbar/2 \,.$$

To derive the time evolution of a Gaussian wave packet we want to start with a momentum distribution centered around $\boldsymbol{k}_0$, i.e.

$$\tilde{\psi}(\boldsymbol{k}, 0) = \left(\frac{a_0^2}{\pi} \right)^{\frac{3}{4}} e^{-\frac{1}{2} a_0 (\boldsymbol{k} - \boldsymbol{k}_0)^2} \,, \quad a_0 \in \mathbb{R} \setminus \{0\}$$
$$\psi(\boldsymbol{x}, 0) = \left(\frac{a_0}{4\pi^3} \right)^{\frac{3}{4}} e^{i a_0^2 \boldsymbol{k}_0 \cdot \boldsymbol{x}} e^{-\boldsymbol{x}^2/2a_0} \,.$$

Using the Schrödinger equation we arrive at

$$\psi(\boldsymbol{x}, t) = \left(\frac{1}{\pi a_0^2 \left(1 + \frac{i\hbar t}{m a_0^2}\right)^2} \right)^{\frac{3}{4}} \times$$
$$\times \exp\left(- \frac{\boldsymbol{x}^2 - 2 i a_0 \boldsymbol{k}_0 \cdot \boldsymbol{x} + i a_0^2 \boldsymbol{k}_0^2 \hbar t/m}{2 a_0^2 \left(1 + \frac{i\hbar t}{m a_0^2}\right)} \right)$$

The probability density is given by

$$\rho(\boldsymbol{x}, t) =$$
$$\left(\frac{1}{\pi^2 a_0^4 \left(1 + \frac{\hbar^2 t^2}{m^2 a_0^4}\right)^2} \right)^{\frac{3}{4}} \exp\left(- \frac{(\boldsymbol{x} - \boldsymbol{v}_0 t)^2}{a_0^2 \left(1 + \frac{\hbar^2 t^2}{m^2 a_0^4}\right)} \right)$$

3 Free particle in big box normalization

One obtains the wave functions

$$\psi_{\boldsymbol{k}}(\boldsymbol{x}) = \frac{1}{L^{3/2}} e^{i \boldsymbol{k} \cdot \boldsymbol{x}}$$

with quantization

$$\boldsymbol{k} = \frac{2\pi}{L} \boldsymbol{n} \,, \quad \boldsymbol{n} \in \mathbb{N}^3 \setminus \{0\}$$

and energy eigenvalues

$$E = \frac{\boldsymbol{p}^2}{2m} = \frac{\hbar^2 \boldsymbol{k}^2}{2m} = \frac{4\hbar^2 \pi^2}{2mL^2} \boldsymbol{n}^2 \,.$$

The density of states is given by

$$\frac{\mathrm{d}N}{\mathrm{d}E} = \frac{m^{3/2} E^{1/2} L^3}{\sqrt{2} \pi^2 \hbar^3} \,.$$

4 Particle in a box

Similar as above, but with the wave functions

$$\psi_{\boldsymbol{k}}(\boldsymbol{x}) = \left(\frac{2}{L} \right)^{\frac{3}{2}} \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

and the limitation $n_x, n_y, n_z \neq 0$. This yields the ground state energy

$$E_{\text{g.s.}} = \frac{6\hbar^2 \pi^2}{mL^2} \,,$$

which is also called the **localization energy**.

Appendices

A Useful relations

$$(a + b)^n = \sum_{k=0}^{n} \binom{n}{k} a^{n-k} b^k$$
$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

A.1 Trigonometry

$$\exp x = \sum_{k=0}^{\infty} \frac{x^k}{k!}$$
$$\sin x = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k+1}}{(2k+1)!}$$
$$\cos x = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k}}{(2k)!}$$

B Stone's theorem

Definition 1.
Let $(\hat{U}_t)_{t\in\mathbb{R}} \subseteq \mathcal{B}(\mathcal{H})$ be a one-parameter family of unitary operators on a Hilbert space $\mathcal{H}$ that is ***strongly continuous****, i.e.*

$$\forall t_0 \in \mathbb{R}\,,\ |\psi\rangle \in \mathcal{H}\ :\ \lim_{t\to t_0} \hat{U}_t\,|\psi\rangle = \hat{U}_{t_0}\,|\psi\rangle\ .$$

and homomorphisms, i.e.

$$\forall s,t \in \mathbb{R}\ :\ \hat{U}_{s+t} = \hat{U}_s\hat{U}_t\,.$$

Then $(\hat{U}_t)_{t\in\mathbb{R}}$ is called ***strongly continuous one-parameter unitary group****.*

There is a one to one correspondence between unitary and hermitian operators in the following sense.

Proposition 3.
Let $(\hat{U}_t)_{t\in\mathbb{R}}$ be a strongly continuous one-parameter unitary group. Then there exists a unique (not necessarily bounded) self-adjoint operator $\hat{G}$ such that

$$\forall t \in \mathbb{R}\ :\ \hat{U}_t = e^{it\hat{G}}\,.$$

Conversely, let $\hat{G}$ be a (not necessarily bounded) self-adjoint operator on a Hilbert space $\mathcal{H}$. Then the one-parameter family $(\hat{U}_t)_{t\in\mathbb{R}}$ of unitary operators defined by

$$\forall t \in \mathbb{R}\ :\ \hat{U}_t := e^{it\hat{G}}$$

is a strongly continuous one-parameter group.

In this case $\hat{G}$ is called the **generator** of the transformation $e^{it\hat{G}}$.

We now also see that, for example, the generator $\hat{\boldsymbol{p}}$ of the translation operator $\hat{T}(\boldsymbol{a}) = e^{-\frac{i}{\hbar}\hat{\boldsymbol{p}}\cdot\boldsymbol{a}}$ is uniquely defined.

Proposition 4 (Residue theorem).

$$\oint_\gamma f(z)\,\mathrm{d}z = 2\pi i \sum_{k=1}^{n} \mathrm{I}(\gamma, a_k)\,\mathrm{Res}(f, a_k)$$

C Proofs

Proof (of 1.5).
$\underline{\Leftarrow}$: Clear.
$\underline{\Rightarrow}$: First, using the properties of the scalar product, we find for an arbitrary operator $\hat{R} : \mathcal{D} \to \mathcal{H}$ the general relation[2] $\forall x, y \in \mathcal{D}$:

$$\begin{aligned}4\langle y, \hat{R}x\rangle =\ &\langle x+y, \hat{R}(x+y)\rangle - \langle x-y, \hat{R}(x-y)\rangle \\ &+ i\langle x+iy, \hat{R}(x+iy)\rangle - i\langle x-iy, \hat{R}(x-iy)\rangle\,.\end{aligned}$$

Setting $\hat{R} = \hat{A} - \hat{B}$ we can rewrite the premise as

$$\forall x \in \mathcal{D} : \langle x, \hat{R}x\rangle = 0$$

and thus, using the general relation, we find

$$\forall x, y \in \mathcal{D} : \langle y, \hat{R}x\rangle = 0\,.$$

Since $\hat{R}x \in \mathcal{D}$ we furthermore have

$$\begin{aligned}&\forall x \in \mathcal{D} : 0 = \langle \hat{R}x, \hat{R}x\rangle = \|\hat{R}x\|^2 \\ \Rightarrow\ &\hat{R} = 0 \quad \Rightarrow \quad \hat{A} = \hat{B}\,.\end{aligned}$$

■

[2]Remember that the scalar product is anti-linear in the first component.