Robertson's derivation of the indeterminacy relation

Heisenberg's indeterminacy relation got in 1929 a precise formulation due to Robertson.

Contents

1. Overview

In his article „Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik"[1] (on the intuitive[1] content of the quantum-theoretical kinematics and mechanics), Werner Heisenberg was the first to derive *indeterminacy relations* between those observable quantities, whose's matrix elements don't have well-defined values at the same time in the quantum-theoretical formalism. He demonstrated, that these relations hold between those quantities, which are not accessible to precise measurements at the same time.

[1] Heisenberg used the notion „anschaulich" and „Anschaulichkeit" not only in the title of his article, but also very often within the text. There is no counterpart for that word in english language. It combines a hint to „intuitive" and something like „visualization".

Heisenberg emphasized — as announced in the title of his article — visualization and intuitive clarity of his considerations. A formally more precise form of the indeterminacy relation was proposed in spring 1929 by Howard Percy Robertson in his article „The Uncertainty Principle“[2]. In the section „Indeterminacy relation“, that relation will be derived as proposed by Robertson. And we will prove that it is valid for arbitrary hermitian operators and arbitrary state functions.

Upfront in the section „Basics“ some fundamental notions of quantum theory are compiled, not least to define the notation which will be used in the sequel. Then in section „Indeterminacy“ a quantitatively exact definition of the indeterminacy of a measurable quantity is presented. This is a purely formal definition; we will not comment on the intricate epistemological and philosophical questions, which are related to that key notion of quantum theory.

2. Basics

2.1. The scalar product of state functions

The state functions $|\psi\rangle$ of quantum theory are elements of a vector space $\mathcal{H}$ over the complex numbers $\mathbb{C}$. They are called state functions, because they contain informations on the state of a physical system. The scalar product S of the state functions is defined as a bi-linear map from $\mathcal{H}$ onto $\mathbb{C}$:

$$\begin{aligned} &S : \mathcal{H} \to \mathbb{C} \\ &S(|\psi\rangle, |\phi\rangle) = \langle\phi|\psi\rangle \in \mathbb{C} \text{ with } |\psi\rangle, |\phi\rangle \in \mathcal{H} \end{aligned} \tag{1}$$

These are important properties of the scalar product (the star* indicates „complex conjugate“):

$$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^* \tag{2a}$$

$$\langle\psi|\psi\rangle \geq 0 \tag{2b}$$

$$\langle\phi|\psi+\chi\rangle = \langle\phi|\psi\rangle + \langle\phi|\chi\rangle \tag{2c}$$

$$\langle\phi|c\psi\rangle = c\langle\phi|\psi\rangle \quad \text{with } c \in \mathbb{C} \tag{2d}$$

$$\langle c\phi|\psi\rangle = c^*\langle\phi|\psi\rangle \quad \text{with } c \in \mathbb{C} \tag{2e}$$

$$\frac{\partial}{\partial x}\langle\phi|\psi\rangle = \langle\frac{\partial\phi}{\partial x}|\psi\rangle + \langle\phi|\frac{\partial\psi}{\partial x}\rangle \tag{2f}$$

Because of (2a), the scalar product of a state function with itself is in any case real:

$$\langle\psi|\psi\rangle = \langle\psi|\psi\rangle^* \in \mathbb{R} \tag{3}$$

Thus (2b) is sensible. Furthermore we prove the Cauchy/Schwarz inequality

$$\langle\psi|\phi\rangle\langle\phi|\psi\rangle = |\langle\psi|\phi\rangle|^2 \leq \langle\psi|\psi\rangle\langle\phi|\phi\rangle \ , \tag{4}$$

which is valid for arbitrary vectors $|\psi\rangle$ and $|\phi\rangle$. In case of $|\psi\rangle = |\phi\rangle$ the inequality holds trivially. Therefore only the case $|\psi\rangle \neq |\phi\rangle$ needs further consideration. Then at most one of the two vectors can be the null-vector (which is the only vector with $\langle 0|0\rangle = 0$). Without loss of generality, we stipulate

$$\langle\phi|\phi\rangle \neq 0 \tag{5}$$

for the following proof. For arbitrary vectors $\in \mathcal{H}$, and for arbitrary $c \in \mathbb{C}$, we have

$$\begin{aligned} 0 &\overset{(2b)}{\leq} \langle\psi + c\phi|\psi + c\phi\rangle \\ 0 &\leq \langle\psi|\psi\rangle + c^*\langle\phi|\psi\rangle + c\langle\psi|\phi\rangle + c^*c\langle\phi|\phi\rangle \ . \end{aligned} \tag{6}$$

Because of $c^*\langle\phi|\psi\rangle \overset{(2a)}{=} (c\langle\psi|\phi\rangle)^*$, we have $(c^*\langle\phi|\psi\rangle + c\langle\psi|\phi\rangle) \in \mathbb{R}$. And of course $c^*c\langle\phi|\phi\rangle \in \mathbb{R}$ holds for the square modulus.

Consequently we may subtract $c^*\langle\phi|\psi\rangle + c\langle\psi|\phi\rangle + c^*c\langle\phi|\phi\rangle$ from both sides of the inequality:

$$-c^*\langle\phi|\psi\rangle - c\langle\psi|\phi\rangle - c^*c\langle\phi|\phi\rangle \leq \langle\psi|\psi\rangle \tag{7}$$

With the definition

$$c \equiv -d \cdot \frac{\langle\phi|\psi\rangle}{\langle\phi|\phi\rangle}\ ,\ c^* \equiv -d^* \cdot \frac{\langle\psi|\phi\rangle}{\langle\phi|\phi\rangle} \quad \text{with } d \in \mathbb{C} \tag{8}$$

we find

$$\begin{aligned} d^*\frac{\langle\psi|\phi\rangle}{\langle\phi|\phi\rangle}\langle\phi|\psi\rangle + d\frac{\langle\phi|\psi\rangle}{\langle\phi|\phi\rangle}\langle\psi|\phi\rangle - d^*\frac{\langle\psi|\phi\rangle}{\langle\phi|\phi\rangle}d\frac{\langle\phi|\psi\rangle}{\langle\phi|\phi\rangle}\langle\phi|\phi\rangle \leq \langle\psi|\psi\rangle \\ (d^* + d - d^*d)\cdot\langle\psi|\phi\rangle\langle\phi|\psi\rangle \leq \langle\psi|\psi\rangle\langle\phi|\phi\rangle\ . \end{aligned} \tag{9}$$

As we want to get the inequality as strong as possible, we look for the maximum $(d^* + d - d^*d)$. Using the definition

$$d \equiv a + ib \quad \text{with } a, b \in \mathbb{R}\ , \tag{10}$$

we find:

$$\begin{aligned} (d^* + d - d^*d) &= a - ib + a + ib - a^2 - b^2 \\ &= 2a - a^2 - b^2 \\ &\text{is maximum for } b = 0 \text{ and } d = a = 1\ . \end{aligned} \tag{11}$$

This proves the Cauchy/Schwarz inequality (4).

2.2. Operators

A map

$$\begin{aligned} A:\ \mathcal{H} \to \mathcal{H} \\ A|\psi\rangle = |\phi\rangle \ \text{ with } |\psi\rangle, |\phi\rangle \in \mathcal{H} \end{aligned} \tag{12}$$

is called an operator. We often will alternatively use this notation:

$$|A\psi\rangle \equiv A|\psi\rangle \tag{13}$$

If the considered system is described by the state vector $|\psi\rangle$, then the expectation value or mean value of the operator A is defined as

$$\langle A\rangle_\psi \equiv \frac{\langle\psi|A\psi\rangle}{\langle\psi|\psi\rangle} \in \mathbb{C} \; . \tag{14}$$

To simplify our formulas, we will in the sequel exclusively use normalized state functions, which are defined by $\langle\psi|\psi\rangle = 1$. Thereby (14) simplifies to

$$\langle A\rangle_\psi \equiv \langle\psi|A\psi\rangle \in \mathbb{C} \; . \tag{15}$$

To each operator A an adjoint operator A^+ is assigned due to the relation

$$\langle A^+\phi|\psi\rangle \equiv \langle\phi|A\psi\rangle \; . \tag{16}$$

2.3. Hermitian operators

In case of $A^+ = A$, the operator A is called self-adjoint or hermitian.

$$\text{Definition:} \quad A \text{ is hermitian} \iff A^+ = A \tag{17}$$

Now we are going to prove: The expectation value of an operator is real for arbitrary state vectors, if and only if the operator is hermitian.

$$\langle A\rangle_\psi \equiv \langle\psi|A\psi\rangle \in \mathbb{R} \; \forall \, |\psi\rangle \in \mathcal{H} \quad \iff \quad A^+ = A \tag{18}$$

First we demonstrate, that the expectation value of an hermitian operator A is necessarily real, by demonstrating that $\langle A\rangle_\psi = \langle A\rangle_\psi^*$ holds:

$$\langle A\rangle_\psi \overset{(15)}{=} \langle\psi|A\psi\rangle \overset{(16)}{=} \langle A^+\psi|\psi\rangle \overset{(17)}{=} \langle A\psi|\psi\rangle \overset{(2a)}{=} \langle\psi|A\psi\rangle^* \overset{(15)}{=} \langle A\rangle_\psi^* \tag{19}$$

In inverse direction, the proof is only slightly more difficult. We must demonstrate that A is hermitian, if it's expectation value is real for arbitrary state functions. For that purpose, we first calculate the expectation value $\langle A\rangle_\chi$ for the state $|\chi\rangle \equiv |\psi\rangle + c|\phi\rangle$ with $c \in \mathbb{C}$:

$$\begin{aligned}\langle A\rangle_\chi &\overset{(15)}{=} \langle\chi|A\chi\rangle \\ &\overset{(2c)}{=} \langle\psi|A\psi\rangle + c^*\langle\phi|A\psi\rangle + c\langle\psi|A\phi\rangle + c^*c\langle\phi|A\phi\rangle\end{aligned} \tag{20}$$

We stipulated $\langle A\rangle_\chi \in \mathbb{R}$ for arbitrary state functions. Thus the first and the fourth term on the right-hand-side of (20) are certainly real. Therefore also the rest of (20) must be real, and consequently identical with it's complex conjugate:

$$\begin{aligned}c^*\langle\phi|A\psi\rangle + c\langle\psi|A\phi\rangle &= c\langle\phi|A\psi\rangle^* + c^*\langle\psi|A\phi\rangle^* \\ &\overset{(2a)}{=} c\langle A\psi|\phi\rangle + c^*\langle A\phi|\psi\rangle\end{aligned} \tag{21}$$

Alternatively, we can write both terms by means of the adjoint operator A^+:

$$c^*\langle\phi|A\psi\rangle + c\langle\psi|A\phi\rangle \overset{(16)}{=} c^*\langle A^+\phi|\psi\rangle + c\langle A^+\psi|\phi\rangle \tag{22}$$

Only if A is hermitian, both (21) and (22) hold at the same time for arbitrary ψ, ϕ, c:

$$\langle A\rangle_\chi \in \mathbb{R} \overset{(21),(22)}{\Longrightarrow} A^+ = A \overset{(17)}{\equiv} A \text{ is hermitian.} \tag{23}$$

2.4. Antihermitian operators

As our last step in preparation for our discussion of the indeterminacy relation, we now will demonstrate that the commutator of two hermitian operators is antihermitian, and it's expectation value is imaginary for arbitrary state functions. For that purpose, we first define what is meant by an antihermitian operator C:

$$\text{Definition:} \quad C \text{ is antihermitian } \Longleftrightarrow C^+ = -C \tag{24}$$

We consider the commutator of two hermitian operators:

$$(AB - BA) \quad \text{with } A^+ = A \text{ and } B^+ = B \tag{25}$$

The expectation value of $(AB - BA)$ for an arbitrary state function $|\psi\rangle$ is

$$\begin{aligned}
\langle\psi|(AB - BA)\psi\rangle &\overset{(2c)}{=} \langle\psi|AB\psi\rangle - \langle\psi|BA\psi\rangle \\
&\overset{(16)}{=} \langle A^+\psi|B\psi\rangle - \langle B^+\psi|A\psi\rangle \\
&\overset{(16)}{=} \langle B^+A^+\psi|\psi\rangle - \langle A^+B^+\psi|\psi\rangle \\
&\overset{(2c)}{=} -\langle(A^+B^+ - B^+A^+)\psi|\psi\rangle \\
&\overset{(25)}{=} -\langle(AB - BA)\psi|\psi\rangle \\
&\overset{(16)}{=} \langle(AB - BA)^+\psi|\psi\rangle \\
&\Longrightarrow \quad (AB - BA)^+ = -(AB - BA)\ .
\end{aligned} \tag{26}$$

Thus the commutator of two hermitian operators is antihermitian. The expectation value of an arbitrary antihermitian operator is imaginary for arbitrary state functions.

$$\begin{aligned}
&\langle C\rangle_\psi = \langle\psi|C\psi\rangle = \langle C^+\psi|\psi\rangle = -\langle C\psi|\psi\rangle = -\langle\psi|C\psi\rangle^* = -\langle C\rangle_\psi^* \\
&\qquad \Longrightarrow \quad \langle C\rangle_\psi \text{ is imaginary, if } C^+ = -C\ .
\end{aligned} \tag{27}$$

3. Indeterminacy

Quantum theory assigns to any observable quantity a hermitian operator. If the operator A is assigned to an observable quantity, and if the considered physical object is in state $|\psi\rangle$, then the mean measured value of that quantity will be the expectation value

$$\langle A\rangle_\psi = \langle\psi|A\psi\rangle \quad \in \mathbb{R}\ . \tag{28}$$

Thereby „mean measured value" indicates, that in general not each measurement will give the result $\langle A\rangle_\psi$. Instead the measurement results will scatter around $\langle A\rangle_\psi$, and only the mean value of many measurements will be equal to $\langle A\rangle_\psi$.

We now are looking for an appropriate expression to quantify how the measured values scatter around the mean value. A poor expression would be the mean deviation from the mean value, because that is zero:

$$\langle A - \langle A\rangle_\psi\rangle_\psi = \langle A\rangle_\psi - \langle\langle A\rangle_\psi\rangle_\psi = \langle A\rangle_\psi - \langle A\rangle_\psi = 0 \tag{29}$$

A much better expression is the mean square deviation:

$$\begin{aligned}\langle\, (A - \langle A\rangle_\psi)^2\,\rangle_\psi &= \langle\, A^2 - 2A\langle A\rangle_\psi + \langle A\rangle_\psi^2\,\rangle_\psi \\ &= \langle A^2\rangle_\psi - 2\langle A\rangle_\psi\langle A\rangle_\psi + \langle A\rangle_\psi^2 \\ &= \langle A^2\rangle_\psi - \langle A\rangle_\psi^2\end{aligned} \tag{30}$$

Therefore we will quantify the scattering ΔA_ψ of the measured values around the mean value in state ψ due to this

$$\text{Definition:}\quad \Delta A_\psi \equiv {}_{+}\!\sqrt{\langle\, (A - \langle A\rangle_\psi)^2\,\rangle_\psi} = {}_{+}\!\sqrt{\langle A^2\rangle_\psi - \langle A\rangle_\psi^2} \tag{31}$$

4. Indeterminacy relation

Let A and B be hermitian operators. We define the hermitian operators

$$A' \equiv A - \langle A\rangle_\psi \quad \text{and} \quad B' \equiv B - \langle B\rangle_\psi \ , \tag{32}$$

and apply the Cauchy/Schwarz inequality (4):

$$\langle A'\psi|A'\psi\rangle\langle B'\psi|B'\psi\rangle \geq \langle A'\psi|B'\psi\rangle\langle B'\psi|A'\psi\rangle = \Big|\langle A'\psi|B'\psi\rangle\Big|^2$$

As the hermitian operators A' and B' are self-adjoint, we may write this inequality as

$$\langle\psi|A'A'\psi\rangle\langle\psi|B'B'\psi\rangle = (\Delta A_\psi)^2(\Delta B_\psi)^2 \geq \Big|\langle A'\psi|B'\psi\rangle\Big|^2 \ . \tag{33}$$

Here (32) has been inserted, and the definition (31) was applied.

According to Pythagoras' theorem, the square modulus of a complex number is equal to the sum of the square modulus of it's real part plus the square modulus of it's imaginary part. Using this theorem, we expand the right-hand-side of (33):

$$\Big|\langle A'\psi|B'\psi\rangle\Big|^2 \overset{(2a)}{=} \langle A'\psi|B'\psi\rangle\langle B'\psi|A'\psi\rangle = \tag{34a}$$
$$= \left|\frac{\langle A'\psi|B'\psi\rangle + \langle B'\psi|A'\psi\rangle}{2}\right|^2 + \left|\frac{\langle A'\psi|B'\psi\rangle - \langle B'\psi|A'\psi\rangle}{2i}\right|^2$$

We first analyze the nominator of the real part:

$$\begin{aligned}
&\langle A'\psi|B'\psi\rangle + \langle B'\psi|A'\psi\rangle = \langle\psi|A'B'\psi\rangle + \langle\psi|B'A'\psi\rangle \overset{(32)}{=} \\
&= \langle\psi|(A-\langle A\rangle_\psi)(B-\langle B\rangle_\psi)\psi\rangle + \langle\psi|(B-\langle B\rangle_\psi)(A-\langle A\rangle_\psi)\psi\rangle = \\
&= \langle\psi|(AB - \langle B\rangle_\psi A - \langle A\rangle_\psi B + \langle A\rangle_\psi\langle B\rangle_\psi|\psi\rangle + \\
&\quad + \langle\psi|(BA - \langle A\rangle_\psi B - \langle B\rangle_\psi A + \langle B\rangle_\psi\langle A\rangle_\psi|\psi\rangle = \\
&= \langle AB + BA\rangle_\psi - 2\,\langle A\rangle_\psi\langle B\rangle_\psi
\end{aligned} \tag{34b}$$

Next we analyze the nominator of the imaginary part of (34a):

$$\begin{aligned}&\langle A'\psi|B'\psi\rangle - \langle B'\psi|A'\psi\rangle = \\ &= \langle\psi|(A-\langle A\rangle_\psi)(B-\langle B\rangle_\psi)\psi\rangle - \langle\psi|(B-\langle B\rangle_\psi)(A-\langle A\rangle_\psi)\psi\rangle = \\ &= \langle AB - BA\rangle_\psi \end{aligned} \tag{34c}$$

Inserting (34) into (33), and computing the positive square root, we get

$$\begin{aligned}&\Delta A_\psi \cdot \Delta B_\psi \geq \\ &\geq \frac{1}{2}\cdot {}_{+}\sqrt{\Big|\langle AB+BA\rangle_\psi - 2\,\langle A\rangle_\psi\langle B\rangle_\psi\Big|^2 + \Big|\langle AB-BA\rangle_\psi\Big|^2}\ .\end{aligned} \tag{35}$$

This form of the indeterminacy relation has been indicated in 1930 by Schrödinger [3].

Robertson started as well from the Cauchy-Schwarz inequality (33), but then he proceeded like this: He assumed that the operators A and B can be written as functions of the operators x, y, z of position and $\frac{\hbar}{i}\frac{\partial}{\partial x}, \frac{\hbar}{i}\frac{\partial}{\partial y}, \frac{\hbar}{i}\frac{\partial}{\partial z}$ of momentum, integrated (33) by parts, and neglected the surface term of his result. Thereby he arrived at

$$\boxed{\Delta A_\psi \cdot \Delta B_\psi \geq \frac{1}{2}\Big|\langle AB-BA\rangle_\psi\Big|}\quad . \tag{36}$$

Obviously we arrive with Schrödinger's simpler and more general method at the same result, by simply neglecting the first square modulus under the root in (35). Let's estimate the value of that term:

$$\begin{aligned}&\Big|\langle AB+BA\rangle_\psi - 2\,\langle A\rangle_\psi\langle B\rangle_\psi\Big| = \\ &\qquad = \Big|\Big\langle AB - \langle B\rangle_\psi A\Big\rangle_\psi - \Big\langle A\langle B\rangle_\psi - BA\Big\rangle_\psi\Big|\end{aligned} \tag{37a}$$

If the commutator $[A,B]=0$, then (37a) is zero, and the right-hand sides of (35) and (36) both are zero. If $[A,B]\neq 0$, then we will in most cases still have

$$\left|\Big\langle AB-\langle B\rangle_\psi A\Big\rangle_\psi-\Big\langle A\langle B\rangle_\psi-BA\Big\rangle_\psi\right|\ll\Big|\langle AB-BA\rangle_\psi\Big|\ . \tag{37b}$$

If we want to have a slightly stronger inequality than Robertson's result (36), then we can of course use Schrödinger's full inequality (35) with no term neglected.

References

[1] W. Heisenberg : *Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik* , Z. Phys. **43**, 172 – 198 (1927), http://dx.doi.org/10.1007/BF01397280 oder: https://www.uni-trier.de/fileadmin/fb1/PHI/Jaeckels_-_Dokumente/Heisenberg_Unbestimmtheitsrelation.pdf english translation: http://ntrs.nasa.gov/search.jsp?R=19840008978

[2] H. P. Robertson : *The Uncertainty Principle* , Phys. Rev. **34**, 163 – 164 (1929), https://doi.org/10.1103/PhysRev.34.163

[3] E. Schrödinger : *Zum Heisenbergschen Unschärfeprinzip*, Sitz. Ber. Preuß. Ak. Wiss., Phys.-Math. **14**, 296 – 303 (1930)