Uncertainty relation for self-adjoint operators

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The uncertainty principle substantiates the notion of incompatibility between two observables by bounding the product of their variations from below by means of the commutator. The correlation coefficient between the observables can be used to obtain an even stronger version.

PRELIMINARIES

Quantummechanical *observables* are represented by self-adjoint operators (on some Hilbert space). Quantummechanical *states* correspond to self-adjoint operators which are additionally positive and have trace 1: $W^\dagger = W \geq 0$ and $\mathrm{Tr}(W) = 1$ (since probabilities are positive and normalized to unity). Moreover, *pure* states are even *projectors* ($W^2 = W$), expressible via state*vectors* $|\psi\rangle$: $W = |\psi\rangle\langle\psi|$. The more general *mixed* states are convex combinations of pure states.

The operation of forming the trace defines a *scalar product* on the Hilbert space $(A;B) := \mathrm{Tr}(A^\dagger B)$. The *expectation value* of an observable A in a state W is given by $\langle A\rangle_W := \mathrm{Tr}(AW) = (A;W)$. Most often the label W in $\langle A\rangle_W$ is left out.

VARIATION AND CORRELATION

The *variation* ΔA of an observable A (in a state W) is defined as

$$\Delta A \;:=\; \sqrt{\left\langle (A - \langle A\rangle)^2 \right\rangle}\,. \tag{1}$$

The correlation coefficient c_{AB} of two observables A and B is defined by

$$c_{AB} \;:=\; \frac{\langle \frac{1}{2}(AB+BA)\rangle - \langle A\rangle\langle B\rangle}{\Delta A\,\Delta B}\,. \tag{2}$$

Since generally A and B need not commute, the symmetrized expression is used in the nominator. Otherwise this definition corresponds exactly to the usual one: covariance divided by the product of the variations. One always has $|c_{AB}| \leq 1$.

CAUCHY-SCHWARZ SAVES THE DAY

Let now A and B be two observables and W a state. We'll first study the special case $\langle A\rangle = \langle B\rangle = 0$. For the square of the variation of A we have

$$\begin{aligned}(\Delta A)^2 &\overset{1}{=} \langle A^2\rangle \overset{2}{=} \mathrm{Tr}(A^2 W) \overset{3}{=} \mathrm{Tr}(AAW^{\frac{1}{2}}W^{\frac{1}{2}}) \\ &\overset{4}{=} \mathrm{Tr}(W^{\frac{1}{2}}A\underbrace{AW^{\frac{1}{2}}}_{\widetilde{A}}) \overset{5}{=} \mathrm{Tr}(\widetilde{A}^\dagger\widetilde{A}) \overset{6}{=} (\widetilde{A};\widetilde{A})\,.\end{aligned} \tag{3}$$

Here, 1 follows from Eqn. (1) and $\langle A\rangle = 0$, 2 from the definition of the expectation value, 3 from the fact that you can take the square root from a positive operator, 4 from the cyclic invariance of the trace, 5 from the self-adjointness of A and W, and finally 6 from the definition of the scalar product.

For the product of the squared variations of A and B we therefore get

$$\begin{aligned}(\Delta A\,\Delta B)^2 &= (\widetilde{A};\widetilde{A})(\widetilde{B};\widetilde{B}) \overset{7}{\geq} |(\widetilde{A};\widetilde{B})|^2 \\ &\overset{8}{=} |\mathrm{Tr}(\widetilde{A}^\dagger\widetilde{B})|^2 \overset{9}{=} |\langle AB\rangle|^2\,.\end{aligned} \tag{4}$$

At the crucial step 7 the *Cauchy-Schwarz inequality* has been used, which holds for positive semi-definite scalar products. Again, 8 is the definition of this scalar product and 9 follows by performing the steps 2, 3, 4 and 5 in reverse order.

THE UNCERTAINTY RELATION

Let us now rewrite the expression $|\langle AB\rangle|^2$:

$$|\langle AB\rangle|^2 \;=\; \left|\frac{1}{2}\langle AB-BA\rangle + \frac{1}{2}\langle AB+BA\rangle\right|^2\,. \tag{5}$$

Since A and B are Hermitian, so is $AB+BA$, and its expectation value must be *real*. However, $AB-BA$ is *anti*-hermitian, with a *purely imaginary* expectation value. Hence, the modulus-squared can be simplified to

$$\begin{aligned}|\langle AB\rangle|^2 &= \frac{1}{4}|\langle AB-BA\rangle|^2 + \frac{1}{4}\langle AB+BA\rangle^2 \\ &\overset{10}{=} \frac{1}{4}|\langle [A,B]\rangle|^2 + c_{AB}^2(\Delta A\,\Delta B)^2\,.\end{aligned} \tag{6}$$

At 10 the definition of the *commutator* $[A,B] := AB - BA$ and the correlation coefficient from Eqn. (2) have been inserted. Together with the inequality (4) this gives

$$\frac{1}{4}|\langle [A,B]\rangle|^2 \;\leq\; (\Delta A\,\Delta B)^2\,(1 - c_{AB}^2)\,, \tag{7}$$

and by taking the square root one finally obtains a strong version of the uncertainty relation:

$$\Delta A\,\Delta B\,\sqrt{1 - c_{AB}^2} \;\geq\; \frac{1}{2}|\langle [A,B]\rangle|\,. \tag{8}$$

This inequality provides a *lower bound* to the product of the variations of two observables A and B. The commutator thus proves to be a suitable measure of incompatibility. If the observables commute, the right hand side is zero and the bound is trivial. Indeed, in this case both observables can both be measured exactly, since the corresponding operators can be diagonalized simultaneously.

Remarkably, for 100% correlated (or anticorrelated) observables (i.e. $c_{AB} = \pm 1$) the left hand side of (8) vanishes. Since the right hand side is clearly nonnegative, the expectation value of the commutator must thus vanish.

Notice that from (7) we also obtain

$$|c_{AB}| \;\leq\; \sqrt{1 - \left| \frac{\langle [A,B] \rangle}{2\,\Delta A\,\Delta B} \right|^2}\,, \tag{9}$$

which for $[A,B] \neq 0$ is a nontrivial bound for the correlation coefficient.

The presented uncertainty relation remains valid for observables with a nonvanishing expectation value, i.e. for noncentered observables which do not satisfy $\langle A \rangle = \langle B \rangle = 0$. This can be seen in the following way: Since $A' := A - \langle A \rangle$ and $B' := B - \langle B \rangle$ are centered by construction, the uncertainty relation (8) holds for them. However, $\Delta A' = \Delta A$ and $\Delta B' = \Delta B$; also, $[A', B'] = [A, B]$ and $c_{A'B'} = c_{AB}$. Therefore the general uncertainty relation follows directly from the one specialized to centered observables – essentially by leaving out the primes.

THE SIMPLER RELATION

The inequality (8) can be softened a bit (but thus made considerably more handy): Since $|c_{AB}| \leq 1$, we also have $0 \leq \sqrt{1 - c_{AB}^2} \leq 1$, and therefore the left hand side of (8) can be be further bounded by

$$\Delta A\,\Delta B \;\;\geq\;\; \frac{1}{2}|\langle [A,B] \rangle|\,. \tag{10}$$

Evidently both inequalities coincide for $c_{AB} = 0$ (i.e. for *uncorrelated* observables).

FINALLY: THE UNCERTAINTY PRINCIPLE

Many textbooks only treat the very special case $A = P$ (momentum) and $B = Q$ (position). Since $[P, Q] = -i\hbar$, relation (10) then yields Heisenberg's traditional uncertainty principle:

$$\Delta P\,\Delta Q \;\;\geq\;\; \frac{\hbar}{2}\,. \tag{11}$$

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