Derivation of the Heisenberg Uncertainty Relation

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1 Preliminaries and Notation

Let's consider a generic state $|\psi\rangle$ and an observable $\hat{O}$ satisfying the following eigenvalues equation:

$$\hat{O}|o_n\rangle = \lambda_n|o_n\rangle$$

Since the observable is Hermitian, we can expand $|\psi\rangle$ as follows:

$$|\psi\rangle = \sum_n a_n|o_n\rangle$$

where $|o_n\rangle$ is the eigenstate of $\hat{O}$ corresponding to the eigenvalue λ_n. According to the *measurement* postulate, after we measure the observable $\hat{O}$ (in the case that no degeneracy occurs) given a quantum system in some state $|\psi\rangle$, as a result we obtain λ_n with a linked probability $|a_n|^2$. Moreover, right after the measurement, the state of the system collapses in the eigenstate $|o_n\rangle$.

The *expectation value* of repeated measurements of $\hat{O}$ on a set of identically prepared states $|\psi\rangle$ is indicated as follows:

$$\langle\hat{O}\rangle_\psi := \langle\psi|\hat{O}|\psi\rangle = \sum_n \lambda_n|\langle o_n|\psi\rangle|^2 \tag{1.1}$$

where $|\langle o_n|\psi\rangle|^2$ represents the probability that the output λ_n will occur.

The measure of the spread of the results around the expectation value is called the *standard deviation* or root-mean-square, i.e. :

$$\begin{aligned}\Delta\hat{O}_\psi &:= \sqrt{\langle(\hat{O} - \langle\hat{O}\rangle)^2\rangle} \\ &= \sqrt{\langle\hat{O}^2\rangle - \langle\hat{O}\rangle^2}\end{aligned} \tag{1.2}$$

Commuting Hermitian operators can be measured simultaneously, i.e. they share a common set of eigenstates in which both operators have a definite value at the same time; simplifying, we can state that two observables $\hat{A}$ and $\hat{B}$ are simultaneously measurable if the result of measuring $\hat{A}$ and then $\hat{B}$ is the same as the one obtained measuring $\hat{B}$ and then $\hat{A}$. In this case the observation of one operator does not affect the observation of the other one, hence the order of the measurements doesn't matter. In the following example we consider two commuting Hermitian operators satisfying the following eigenvalue equations:

$$\hat{A}|\psi_n\rangle = \alpha_n|\psi_n\rangle$$
$$\hat{B}|\psi_n\rangle = \beta_n|\psi_n\rangle$$

where $\{|\psi_n\rangle\}$ are a complete set of common eigenstates with respect to the eigenvalues $\{\alpha_n\}, \{\beta_n\}$ In Fig. 1 and Fig. 2 there are represented two simple examples of measurements of commuting and non-commuting operators. The Δt are taken small enough to preserve the state from changes occuring during the time evolution. This example can be generalized to deal with more than two observables considering also the case in which degeneracy occurs.

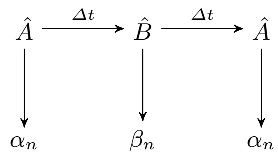

Fig. 1: Measurement of commuting observables

On the contrary, in the case of two operators that do not commute, i.e. their commutator has a non-zero value, it does not exist a complete set of common eigenstates, hence performing a measurement on them simultaneously is not possible. Moreover, the measurement of one operator affects the measurement of the other one, hence the order of the measurements is important.

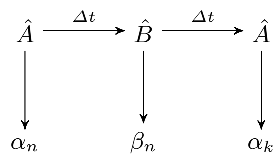

Fig. 2: Measurement of non-commuting observables

In Fig. (2) the two outcomes α_n and α_k are not necessarily the same. We will see that the existence of non-commuting observables is at the basis of the Heisenberg's uncertainty relation and is a quite important physical result. To derive the uncertainty relation we will use the *Schwarz Inequality*:

$$\langle\varphi|\varphi\rangle\langle\psi|\psi\rangle \geq |\langle\varphi|\psi\rangle|^2 \tag{1.3}$$

with equality holding when $|\psi\rangle = \alpha|\varphi\rangle$, for any two normalized states $|\varphi\rangle, |\psi\rangle$ in a Hilbert space $\mathcal{H}$.

2 Derivation

At first we will derive the uncertainty relation for a generalized pair of non-commuting Hermitian operators.

Let $\hat{A}$ and $\hat{B}$ be two non-commuting Hermitian operators, i.e. $[\hat{A}, \hat{B}] \neq 0$. We will prove that the following inequality holds:

$$\varDelta\hat{A}_\psi \varDelta\hat{B}_\psi \geq \frac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle_\psi| \tag{2.1}$$

To make the calculations easier we will express the latter inequality in term of variance, i.e.:

$$(\varDelta\hat{A})^2(\varDelta\hat{B})^2 \geq \frac{1}{4}|\langle[\hat{A}, \hat{B}]\rangle|^2 \tag{2.2}$$

Proof. Before starting the derivation of the uncertainty relation, we need some extra definitions.

Let $\hat{A}'$ and $\hat{B}'$ be two non-commuting Hermitian operators defined as follows:

$$\hat{A}' := \hat{A} - \langle\hat{A}\rangle \tag{2.3a}$$

$$\hat{B}' := \hat{B} - \langle\hat{B}\rangle \tag{2.3b}$$

that, when acting on the state $|\psi\rangle$ give, respectively:

$$\hat{A}'|\psi\rangle := |\psi_{A'}\rangle \tag{2.4a}$$

$$\hat{B}'|\psi\rangle := |\psi_{B'}\rangle \tag{2.4b}$$

We can easily verify that the commutator of these operators is equal to the commutator between $\hat{A}$ and $\hat{B}$:

$$\begin{aligned}[\hat{A}', \hat{B}'] &= [(\hat{A} - \langle\hat{A}\rangle)(\hat{B} - \langle\hat{B}\rangle)] - [(\hat{B} - \langle\hat{B}\rangle)(\hat{A} - \langle\hat{A}\rangle)] \\ &= [\hat{A}, \hat{B}]\end{aligned} \tag{2.5}$$

We can write the product between $\hat{A}'$ and $\hat{B}'$ in the following way:

$$\begin{aligned}\hat{A}'\hat{B}' &= \frac{1}{2}\hat{A}'\hat{B}' + \frac{1}{2}\hat{A}'\hat{B}' + \frac{1}{2}\hat{B}'\hat{A}' - \frac{1}{2}\hat{B}'\hat{A}' \\ &= \frac{1}{2}(\hat{A}'\hat{B}' + \hat{B}'\hat{A}') + \frac{1}{2}(\hat{A}'\hat{B}' - \hat{B}'\hat{A}') \\ &= \frac{1}{2}\{\hat{A}', \hat{B}'\} + \frac{1}{2}[\hat{A}', \hat{B}']\end{aligned} \tag{2.6}$$

This way we have decomposed the above product in an anti-Hermitian part, i.e., $[\hat{A}, \hat{B}]^\dagger = -[\hat{A}, \hat{B}]$ and in an Hermitian one, i.e., $\{\hat{A}, \hat{B}\}^\dagger = \{\hat{A}, \hat{B}\}$.

Now we can give the proof of the inequality as expressed in Eq. (2.2).

$$\begin{aligned}(\Delta\hat{A})^2(\Delta\hat{B})^2 &= \langle\psi|(\hat{A}-\langle\hat{A}\rangle)^2|\psi\rangle\langle\psi|(\hat{B}-\langle\hat{B}\rangle)^2|\psi\rangle \\ &= \langle\psi|(\hat{A}')^2|\psi\rangle\langle\psi|(\hat{B}')^2|\psi\rangle \\ &= \langle\psi_{A'}|\psi_{A'}\rangle\langle\psi_{B'}|\psi_{B'}\rangle \end{aligned} \tag{2.7}$$

The last equality follows from the hermiticity of $\hat{A}'$ and $\hat{B}'$. Using the *Schwarz Inequality* we obtain:

$$\begin{aligned}\langle\psi_{A'}|\psi_{A'}\rangle\langle\psi_{B'}|\psi_{B'}\rangle \geq |\langle\psi_{A'}|\psi_{B'}\rangle|^2 &= |\langle\psi|\hat{A}'\hat{B}'|\psi\rangle|^2 \\ &= |\langle\psi|\frac{1}{2}\{\hat{A}',\hat{B}'\}+\frac{1}{2}[\hat{A}',\hat{B}']|\psi\rangle|^2 \\ &\geq \frac{1}{4}|\langle\psi|[\hat{A}',\hat{B}']|\psi\rangle|^2 \end{aligned} \tag{2.8}$$

The decomposition in Eq. (2.6) implies a decomposition also for the mean values of the aforementioned product. Moreover, from the hermiticity of $\hat{A}'$ and $\hat{B}'$ it follows that $\langle\psi|\{\hat{A}',\hat{B}'\}|\psi\rangle$ is real, while $\langle\psi|[\hat{A}',\hat{B}']|\psi\rangle$ is a pure imaginary number [1], hence the anti-commutator only strengthens our inequality because the modulus of a complex number is always greater than the modulus of its imaginary part only. If we substitute this result in the Eq. (2.7) we can prove that the inequality in Eq. (2.2) holds:

$$\begin{aligned}(\Delta\hat{A})^2(\Delta\hat{B})^2 &= \langle\psi|(\hat{A}')^2|\psi\rangle\langle\psi|(\hat{B}')^2|\psi\rangle \\ &\geq \frac{1}{4}|\langle\psi|[\hat{A}',\hat{B}']|\psi\rangle|^2 = \frac{1}{4}|\langle\psi|[\hat{A},\hat{B}]|\psi\rangle|^2 \end{aligned} \tag{2.9}$$

Taking the square root of the last inequality we obtain:

$$\Delta\hat{A}_\psi\Delta\hat{B}_\psi \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle_\psi| \tag{2.10}$$

□

Recall that the equality holds when $|\psi_{A'}\rangle = k|\psi_{B'}\rangle$, and the coefficient k is a pure imaginary number such that $k = i\alpha$ with $\alpha \in \mathbb{R}$. We need k to be purely imaginary due to the fact that the mean value in the right part of the Eq. (2.10) is purely imaginary and we don't want any of the considered expectation values to be zero.

We will use this in the following to find the states which minimize the uncertainty.

2.1 Uncertainty relations for Position and Momentum operators

Let's now consider the uncertainty relation for the case in which we take:

$$\hat{A} = \hat{q}$$
$$\hat{B} = \hat{p}$$

[1] The expectation value of an anti-Hermitian operator is $\langle\hat{O}\rangle = -\langle\hat{O}\rangle^*$.

where $\hat{q}$ and $\hat{p}$ are, respectively, the position and momentum operators. We want to prove that the following inequality holds:

$$\Delta\hat{q}\Delta\hat{p} \geq \frac{\hbar}{2} \tag{2.11}$$

This case is more interesting than the generalized one since the right part of the inequality does not depend on the state $|\psi\rangle$ of the system. The commutator between $\hat{q}$ and $\hat{p}$ is:

$$[\hat{q}, \hat{p}] = i\hbar \tag{2.12}$$

Substituting such commutator we obtain the following inequality:

$$\begin{aligned}(\Delta\hat{q})^2(\Delta\hat{p})^2 \geq \frac{1}{4}|\langle[\hat{q}, \hat{p}]\rangle|^2 &= \frac{1}{4}|\langle i\hbar\rangle|^2 \\ &= \frac{\hbar^2}{4}\end{aligned} \tag{2.13}$$

which implies that the (2.11) inequality holds. We can interpret this as a lower bound on the accuracy by which we can know both the position and the momentum of a particle given a state $|\psi\rangle$. Hence, once the lower bound is reached, the smaller is the variance of the position the higher is the uncertainty for the momentum and vice-versa.

2.2 Minimum uncertainty states for $\hat{q}$ and $\hat{p}$

It is possible to build states having the minimum possible spread of $\hat{p}$ and $\hat{q}$, i.e., states that make the inequality in (2.11) become an equality:

$$\Delta\hat{q}\Delta\hat{p} = \frac{\hbar}{2} \tag{2.14}$$

This equality holds if and only if the two vectors involved are proportional to each other. Moreover, as we have already seen above, we require that the coefficient of proportionality is a complex number with the imaginary part only.

$$[\hat{q} - \langle\hat{q}\rangle]|\psi\rangle = k[\hat{p} - \langle\hat{p}\rangle]|\psi\rangle \qquad \textit{where } k = i\alpha$$

The latter equation, as we have used the coordinate representation, becomes:

$$[q - \langle\hat{q}\rangle]\psi(q) = i\alpha[-i\hbar\frac{d}{dq} - \langle\hat{p}\rangle]\psi(q) \tag{2.15}$$

We can re-write it as:

$$\alpha\hbar\frac{d}{dq}\psi(q) - q\psi(q) + (\langle\hat{q}\rangle - i\alpha\langle\hat{p}\rangle)\psi(q) = 0$$

Which can be simplified as follows:

$$\begin{aligned}
\alpha\hbar\frac{d}{dq}\psi &= \psi(q - \langle\hat{q}\rangle + i\alpha\langle\hat{p}\rangle) \\
\Rightarrow \int \frac{d\psi}{\psi} &= \int \frac{q + i\alpha\langle\hat{p}\rangle - \langle\hat{q}\rangle}{\alpha\hbar}\, dq \\
\Rightarrow \ln\psi &= \frac{q^2}{2\alpha\hbar} + \frac{i\langle\hat{p}\rangle q}{\hbar} - \frac{\langle\hat{q}\rangle q}{\alpha\hbar} + C. \\
&= \frac{q^2 - 2\langle\hat{q}\rangle q + \langle\hat{q}\rangle^2 - \langle\hat{q}\rangle^2}{2\alpha\hbar} + i\frac{\langle\hat{p}\rangle q}{\hbar} + C. \\
\Rightarrow \psi(q) &= A\exp\Big[\frac{(q - \langle\hat{q}\rangle)^2}{2\alpha\hbar} + \frac{i\langle\hat{p}\rangle q}{\hbar} - \frac{\langle\hat{q}\rangle^2}{2\alpha\hbar}\Big] \qquad (2.16)
\end{aligned}$$

Where A is a constant to be determined by normalizing the state. Eq. (2.16) represents the form of minimum uncertainty states that, as we can see, take the standard Gaussian form.

Step-by-step Wavefunction Normalization

In the following we made a step-by-step normalization of the wavefunction $\psi(q)$ for those who are not familiar with it. As it is a Gaussian function it looks difficult if you are not trained, so I decided to display all the calculations here. Recall that A is in the form e^C and $\alpha \leq 0$.

$$\int_{-\infty}^{+\infty} |\psi(q)|^2 dq = 1$$

Now let's expand it:

$$\int_{-\infty}^{+\infty} |Ae^{(\frac{(q-\langle\hat{q}\rangle)^2}{2\alpha\hbar} + \frac{i\langle\hat{p}\rangle q}{\hbar} - \frac{\langle\hat{q}\rangle^2}{2\alpha\hbar})}|^2 dq = 1$$

We can now take $|A|^2$ out of the integral (remember that $A = e^C$) and rewrite the modulus square that remains inside the integral in this way:

$$|A|^2 \int_{-\infty}^{+\infty} e^{(\frac{(q-\langle\hat{q}\rangle)^2}{2\alpha\hbar} + \frac{i\langle\hat{p}\rangle q}{\hbar} - \frac{\langle\hat{q}\rangle^2}{2\alpha\hbar})} e^{(\frac{(q-\langle\hat{q}\rangle)^2}{2\alpha\hbar} - \frac{i\langle\hat{p}\rangle q}{\hbar} - \frac{\langle\hat{q}\rangle^2}{2\alpha\hbar})} dq = 1$$

We can simplify the terms $\frac{i\langle\hat{p}\rangle q}{\hbar}$ and $-\frac{i\langle\hat{p}\rangle q}{\hbar}$ and make the remaining calculations, obtaining:

$$|A|^2 \int_{-\infty}^{+\infty} e^{(\frac{(q-\langle\hat{q}\rangle)^2}{\alpha\hbar} - \frac{\langle\hat{q}\rangle^2}{\alpha\hbar})} dq = 1$$

The term $\frac{\langle\hat{q}\rangle^2}{2\alpha\hbar}$ is a constant, you can see that it does not depend from q, so now we have an integral in the form $\int_{-\infty}^{+\infty} e^{-ax^2+bx+c}$ that we are able to solve[2] and

[2] if you are not able to solve it check here **link**

the result is:

$$|A|^2\sqrt{\frac{\pi}{\frac{1}{|\alpha|\hbar}}}\; e^{-\frac{\langle\hat{q}\rangle^2}{\alpha\hbar}} = |A|^2\sqrt{\pi|\alpha|\hbar}\; e^{-\frac{\langle\hat{q}\rangle^2}{\alpha\hbar}} = 1$$

Now it's trivial to determine the value of A:

$$|A|^2 = e^{\frac{\langle\hat{q}\rangle^2}{\alpha\hbar}}\; \frac{1}{\sqrt{\pi|\alpha|\hbar}}$$

$$A = e^{\frac{\langle\hat{q}\rangle^2}{2\alpha\hbar}}\; \frac{1}{\sqrt[4]{\pi|\alpha|\hbar}}$$

And the value of the wavefunction $\psi(q)$:

$$\psi(q) = \frac{1}{\sqrt[4]{\pi|\alpha|\hbar}}\; e^{\frac{\langle\hat{q}\rangle^2}{2\alpha\hbar}}\; e^{\left(\frac{(q-\langle\hat{q}\rangle)^2}{2\alpha\hbar}+\frac{i\langle\hat{p}\rangle q}{\hbar}-\frac{\langle\hat{q}\rangle^2}{2\alpha\hbar}\right)}$$

$$= \frac{1}{\sqrt[4]{\pi|\alpha|\hbar}}\; e^{-\frac{(q-\langle\hat{q}\rangle)^2}{2|\alpha|\hbar}+\frac{i\langle\hat{p}\rangle q}{\hbar}}$$