The expression of the Uncertainty Principle of Quantum Mechanics

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Overview

1. Introduction: The early history of the uncertainty principle: from a semi-quantitative and ambiguous formulation (1927) to the adoption of a precise inequality: the standard uncertainty relation (1930).
2. A problem for this standard uncertainty relation: the single slit experiment.
3. Conceptually stronger uncertainty relations that overcome this problem. Landau & Pollak and the entropic uncertainty relations.
4. A second problem: the double slit experiment.
5. An approach that overcomes this second problem.
6. Conclusions

Based on joint work with Jan Hilgevoord in the 1980's and 1990's.

Jan Hilgevoord (1927 - 2025)

1. Introduction

- In 1927, Werner Heisenberg introduced his famous Uncertainty Principle in Quantum Mechanics.
- The purpose of his paper was to provide intuitive understanding for the "Matrix Mechanics" version of Quantum Mechanics that he had developed in 1925 (with Born and Jordan).
- In particular, he argued that any attempt to define a dynamical quantity of a quantum system (say: the postion of an electron) required the specification of an experiment in which this quantity can be measured.
- By analyzing a thought-experiment (the γ-ray microscope) in which the position of an electron could be measured precisely, he concluded that:
  [T]he more precisely the position of the electron is determined, the less precisely its momentum is known and conversely.
- He expressed this by a semiquantitative relation

$$\delta p \delta q \sim h$$

1. Introduction

- In his 1927 paper (and other papers he wrote in 1927-1929), he did not define exactly what the "δ's " in this relation meant or how they were defined. (*"etwa die mittlere Fehler"*).
- Instead, he referred to "δq" etc. as "imprecision", "uncertainty", "inaccuracy", "unsharpness" etc., and chose some characteristic measure to quantify them, different for each example discussed.
- However, still in the same year (1927), E.H. Kennard proved a general theorem of quantum mechanics:
  Let P and Q be the self-adjoint operators for momentum and postion, and $|\psi\rangle$ any quantum state (i.e. a unit vector in Hilbert space), then

$$\Delta_\psi P \Delta_\psi Q \geq \frac{\hbar}{2} \tag{1}$$

  Where $\Delta_\psi P := \left(\langle\psi|P^2|\psi\rangle - \langle\psi|P|\psi\rangle^2\right)^{1/2}$ denotes a standard deviation.

1. Introduction

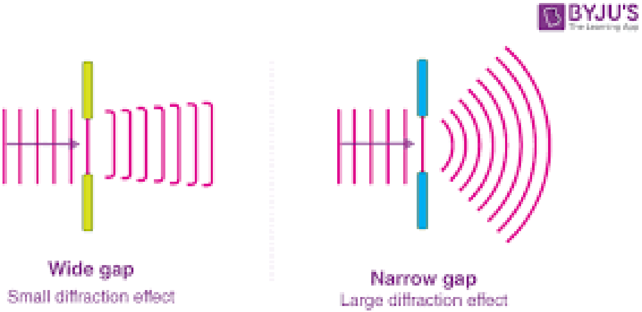
- In 1929 H.P. Robertson extended Kennard's result by showing that for any two quantum observables, represented by the self-adjoint operators A and B:, the following inequality holds:

$$\Delta_\psi A \Delta_\psi B \geq \frac{1}{2} |\langle\psi|[A, B]|\psi\rangle| \quad (2)$$

- While Kennard had not remarked on the question why the standard deviation would be an appropriate choice, Robertson's only comment was that this choice was "in accordance with statistical usage".
- In the book *Physical Principles of Quantum Theory* (1930), Heisenberg explicitly endorsed Kennard's inequality and argued that "this proof does not differ at all in mathematical content" form his own semi-quantitative argument of 1927, the only difference being that "now the proof is carried through exactly".

1. Introduction

- So, the upshot is that within a few years the physical community agreed that the inequality $\Delta_\psi P \Delta_\psi Q \geq \frac{\hbar}{2}$ was seen as the exact expression of Heisenberg's Uncertainty Principle. I will call it the *standard uncertainty relation*.
- But is that view correct? Let us look at one of Heisenberg's own illustrations of the Uncertainty Principle: the diffraction through a single slit.



Problem: single slit diffraction

- One example Heisenberg discussed explicitly in his (1930) book is the diffraction by quantum systems through a narrow slit.

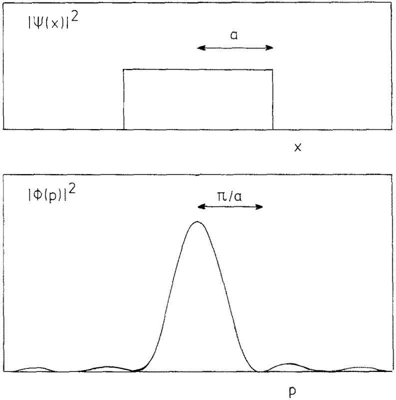


Fig. 2. The probability density of position and momentum at the screen for the single-slit experiment.

2. A Problem: the single-slit experiment

- This example is meant to illustrate that the narrower the slit is that a beam of particles has to go through; the wider the diffraction pattern becomes behind the slit (indicating a loss in precision in predicting their momentum).
- To express this quantitatively, all textbook discussions of this example do not rely on the standard deviations in the standard uncertainty relation; instead, they express the uncertainty in position as determined by the slit width a, and the width of the diffraction pattern by the distance between the main maximum and the first minimum. This gives

$$\delta q = 2a, \quad \delta p = \frac{\pi\hbar}{a}, \quad \text{so that:} \quad \delta q \delta p = 2\pi\hbar = h \qquad (3)$$

- But what if we used standard deviations? The result would be

$$\Delta_\psi Q = a/\sqrt{3}, \quad \Delta_\psi P = \infty, \quad \text{and so: } \Delta_\psi P \Delta_\psi Q = \infty \qquad (4)$$

- This, of course, does not violate the standard uncertainty relation, but fails to express the intended reciprocity between slit width and width of the diffraction pattern.

Diagnosis

- What goes wrong is that a standard deviation, like $\Delta_\psi P$, is dominated by a term
$$\int p^2 |\tilde{\psi}(p)|^2 \, dp.$$
When $|\tilde{\psi}(p)|^2 \propto \frac{\sin^2 ap}{(ap)^2}$, its tails drop off like p^{-2}, so this term blows up.
- Now, the fact that $\Delta_\psi P$ diverges here, is not the problem. It could readily be avoided by smoothing the edges of the slit a little bit. In that case, $\Delta_\psi P$ will be finite; but its value would still depend on the amount of smoothing, and not on the slit width, as required.
- The objection to the standard deviation as a measure of uncertainty is rather that, for any $\epsilon > 0$, it is possible to have a fraction of $1 - \epsilon$ of a probability distribution concentrated in an interval as small as you like, while keeping the standard deviation as large as you like.
- So we need other expressions for uncertainty than the standard deviation.

3. Overcoming this problem: (i) Landau and Pollak

- One way to attempt to find a better expression for uncertainty would be to look for the size of an interval on which the main bulk (say: 90%) of the probability distribution is contained. This is an approach developed by H.J.Landau & H.O.Pollak of Bell Systems Lab in 1961.
- In more detail, pick a value $0 \leq \alpha < 1$ and let

$$W_\alpha(Q,\psi) := \inf_{|I|} \left\{ |I| \ : \ \int_I |\psi(q)|^2 \, dq = \alpha \right\} \tag{5}$$

be the size of the smallest interval on which a portion α of the total probability for the position Q in state $|\psi\rangle$ is concentrated. Similarly, define:

$$W_\beta(P,\psi) := \inf_{|I|} \left\{ |I| \ : \ \int_I |\tilde{\psi}(p)|^2 \, dp = \beta \right\} \tag{6}$$

Landau & Pollak proved the uncertainly relation (if $\alpha + \beta \geq \frac{1}{2}$):

$$W_\alpha(Q,\psi) W_\beta(P,\psi) \geq 2\pi\hbar \left(\alpha\beta - \sqrt{(1-\alpha)(1-\beta)} \right)^2 \tag{7}$$

Comments on Landau & Pollak

- First of all, the definition of a "bulk width" like $W_\alpha(Q,\psi)$ is not dependent on the tail behaviour of the probability distribution. Moreover, it is finite for all quantum states $|\psi\rangle$ (as long as $\alpha < 1$). It therefore does not run into the problems we encountered for standard deviations.
- Furthermore, bulk widths are conceptually stronger than standard deviations in the sense that the bulk width implies a lower bound on the corresponding standard deviation but not vice versa. In fact, the classical Bienaymé-Chebyshev inequality (quite independent of quantum theory) implies

$$W_\alpha(Q,\psi) \leq \frac{2}{\sqrt{1-\alpha}} \Delta_\psi Q \tag{8}$$

  So, the Landau-Pollak relation by itself implies the existence of a lower bound on the product of standard deviations (but not quite the optimal lower bound).

Overcoming this problem (ii): Entropic uncertainty relations

- Another approach, due to Beckner (1975) and Białinicki-Birula & Micielski (1975), is to use a continuous version of the Shannon entropy of a probability distribution:

$$H(Q,\psi) := -\int \ln|\psi(q)|^2 |\psi(q)|^2 dq \tag{9}$$

- Although expressions like this are well-known, especially in information theory, their application to probability distributions over a continuum has some conundrums: in particular, they are not always non-negative, and carry a physical dimension (for position) of $\ln[m]$. Both conundrums can be removed by simply taking an exponent.
- The result of the above authors is

$$H(Q,\psi) + H(P,\psi) \geq \ln(e\pi\hbar) \quad \text{or} \quad e^{H(Q,\psi)} e^{H(P,\psi)} \geq e\pi\hbar \tag{10}$$

Comments on the entropic uncertainty relations

- The entropic uncertainty relation almost overcomes the objection we raised against the standard deviation: It can still happen that $H(Q, \psi)$ becomes as large as one likes, while $1 - \epsilon$ of the total probability is concentrated in an arbitrarily small interval, but admittedly in rather far-fetched cases.
- It strictly implies the standard uncertainty relation, since, independently of quantum theory:

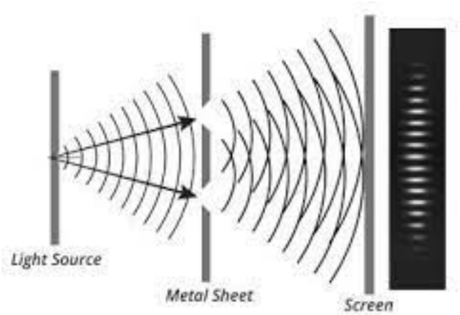
$$-\int \ln \psi(q)|^2 |\psi(q)|^2 dq \leq \ln(\sqrt{(}2\pi e \Delta_\psi Q) \tag{11}$$

so that

$$\frac{\hbar}{2} \leq \frac{1}{2\pi e} e^{H(Q,\psi)+H(P,\psi)} \leq \Delta_\psi Q \delta_\psi P \tag{12}$$

4. The double slit experiment

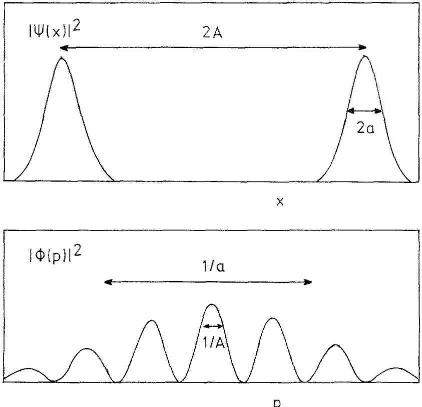
- Another thought experiment that played a crucial role in the debate on the interpretation of Quantum Mechanics is the double slit experiment.
- Particularly well-known is the discussion between Einstein and Bohr (1927) about whether it would be possible to measure through which slit a quantum particle travels without disturbing the interference pattern. Bohr famously employed the Uncertainty Principle to argue that this was impossible.



- In this case, there are two parameters: a: the slit width; A: the distance between the slits, with $a << A$.
- Furthermore we see from the figure that there are two kinds of reciprocal relations here

$$\text{fine width in position:} \quad a \quad \longleftrightarrow \quad \text{overall width in momentum:} \quad \frac{1}{a}$$

$$\text{fine width in momentum:} \quad \frac{1}{A} \quad \longleftrightarrow \quad \text{overall width in position:} \quad A$$



- It is this second reciprocal relationship (between the fine width in momentum and bulk width in position that underlies Bohr's argument that the Uncertainty Principle implies that any attempt to determine through which slit a particle travels will wash out the fine interference structure.
- But obviously, all the measures of uncertainty we discussed so far (the standard deviation, the bulk width W, and the entropic measure are all insensitive to the presence or absence of this interference structure in the wave function; i.e. for the momentum wave function in this example they all have values proportional to $1/a$, rather than $1/A$.
- So, I claim that in order to express this application of the Uncertainty Principle, we also need a measure of uncertainty that is sensitive to presence of fine structure in a wave function.

5. Overcoming this second problem

- A way to find such a measure (say, for a position wave function $\psi(q)$) is to consider the overlap (or autocorrelation) integral between this wave function and a copy that has been displaced over some distance a:

$$I(a) := \left| \int \psi^*(q)\,\psi(q-a)\,dq \right| \tag{13}$$

  Intuitively, if ψ has fine structure, $I(a)$ will decrease rapidly from its unique maximum $I(0) = 1$ for small values of a (perhaps showing increases for larger a by overlap of cross-terms). If ψ does not have any fine structure, the decay of $I(a)$ as a function of parameter a will only decrease slowly for small values of a
- Thus, we may find an interesting measure for fine structure width by looking at how fast $I(a)$ decreases for small values of a.
- So, let us pick a value $0 < \gamma < 1$ and define the translation width of ψ as:

$$w_\gamma(Q,\psi) := \inf_{a>0}\{a \ : \ \left| \int \psi^*(q)\psi(q-a)\,dq \right| = \gamma\} \tag{14}$$

- It is not difficult to show that $w_\gamma(Q,\psi) \leq W_\alpha(Q,\psi)$ for $\alpha^2 + \gamma^2 \geq 1$. Also, $w_\gamma(Q,\psi)$ bounds the standard deviation $\Delta_\psi Q$, due to a result of Levy-Leblond:

$$|\int \psi^*(q)\psi(q-a)\,dq|^2 \leq \left(1 + (\frac{a}{\Delta_\psi Q})^2\right)^{-1} \tag{15}$$

  So, w is indeed a more sensitive measure than W or Δ.
- When it comes to uncertainty relations, a first result (that is actually quite well-known) is that the behaviour of the autocorrelation function for small a is bounded by

$$|\int \psi^*(q)\psi(q-a)\,dq| \geq \cos \hbar^{-1} a \Delta_\psi P \tag{16}$$

  It follows from this that

$$w_\gamma(Q,\psi)\Delta_\psi P \geq 2\hbar \arccos\gamma \tag{17}$$

- But since the standard deviation is not a satisfactory expression of uncertainty, a more appealing result is

$$w_\gamma(Q,\psi) W_\alpha(P,\psi) \geq 2\hbar \arccos \frac{\alpha + 1 - \gamma}{\gamma} \quad \text{if} \quad \gamma \leq 2\alpha - 1 \tag{18}$$

An objection

- An objection that has been raised is that our definition of w is not a measure of position uncertainty at all, because it relies on the autocorrelation integral of the position wave function

$$\int \psi^*(q)\psi(q-a)dq = \langle\psi|U(a)|\psi\rangle$$

where $U(a)$ is the displacement or translation operator $U(a) : \psi(q) \mapsto U(a)\psi(q) = \psi(q-a)$. In quantum theory, this translation operator is generated by momentum, i.e, $U(a) = e^{iaP}$, we could equivalently write

$$\int \psi^*(q)\psi(q-a)dq = \langle\psi|U(a)|\psi\rangle = \int e^{iap}|\tilde{\psi}(p)|^2\,dp$$

So why should one think of this integral as providing a measure of uncertainty in position rather than momentum, when in fact, it is a functional on the momentum probability distribution $|\tilde{\psi}(p)|^2$?

- the easiest answer is of course that

$$|\int \psi^*(q)\psi(q-a)\,dq| \leq \int |\psi(q)\psi(q-a)|\,dq$$

so that the autocorrelation integral does have implications for how the position probability distribution $|\psi(q)|^2$ behaves.
- A more informative answer can be obtained by drawing a connection to the theory of statistical inference.

Statistical Inference

- Consider the classical statistical problem of estimating a real parameter θ in a family of probability distributions $p_\theta(x)$. The technique that is often employed is to construct a function $\tau(x)$, an *estimator*, that is intended to estimate the value of θ. A famous result that bounds the standard deviation $\Delta_\theta \tau$ for all unbiassed estimators $(\langle\tau\rangle\theta = \theta)$ is the Cramér-Rao Inequality:

$$\Delta_\theta \tau \geq \left(\int \frac{1}{p_\theta(x)} \left(\frac{dp_\theta(x)}{d\theta} \right)^2 dx \right)^{-1/2} \tag{19}$$

Where the integral on the right-hand side is known as the Fisher information.
If we generalize this to the case of multiple parameters $\vec{\theta} = (\theta_1, \ldots, \theta_n)$, this Fisher information becomes a tensor

$$I_{ij} = \int \frac{1}{p_{\vec{\theta}}(x)} \frac{\partial p_{\vec{\theta}}(x)}{\partial \theta_i} \frac{\partial p_{\vec{\theta}}(x)}{\partial \theta_j} dx \tag{20}$$

- This tensor can in fact be seen as a metrical tensor that generates a distance between probability distributions: the statistical distance. It can be shown that it generates the distance

$$d(p,q) := \arccos \int \sqrt{p(x)q(x)}dx. \tag{21}$$

Applying this in quantum theory, suppose we want to estimate the parameter a in a family of quantum states $\{\psi_a \;:\; \psi_a(q) = \psi(q-a)\}$. This time, we are not restricted to using real-valued functions as estimator, we can use any self-adjoint operator. We find by a similar argument (choosing the most discriminating observable) that the statistical distance between two states of this family is

$$d(\psi,\psi_a) = \arccos \left| \int \psi^*(q)\psi(q-a)dq \right| \tag{22}$$

This means that $w(Q,\psi)$ bounds, not just the standard deviation ΔQ, but that of any unbiased observable that is sensitive to the location of the state within this family.

6. Conclusions and remarks

- A satisfactory of expression of the Uncertainty Principle takes a lot more than just the usual standard uncertainty relation.
- Conceptually, the translation width $w_\gamma(Q, \psi)$ stands apart from the other expressions: instead of measuring the spread of the quantum probability distribution over the possible values of the position operator Q, it can be interpreted as a bound to how well a location parameter in a family of quantum states can be estimated (by any measurement). It is not dependent on the existence of the position operator Q, and indeed is also well defined for quantities for which the existence of a self-adjoint position operator is problematic.
- Indeed, this last approach the the uncertainty principle can also straightforwardly be applied to the case of energy and time, and other versions of the uncertainty principle where there is no general self-adjoint operator for one of the variables involved.

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