Matrices and Uncertainty

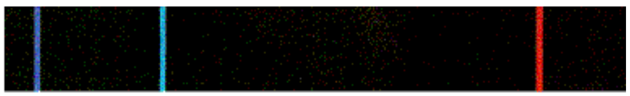
8.225 / STS.042, Physics in the 20th Century
Professor David Kaiser, 7 October 2020

1. Quantum Numbers and Spin

2. Heisenberg and Matrix Mechanics

3. The Uncertainty Principle

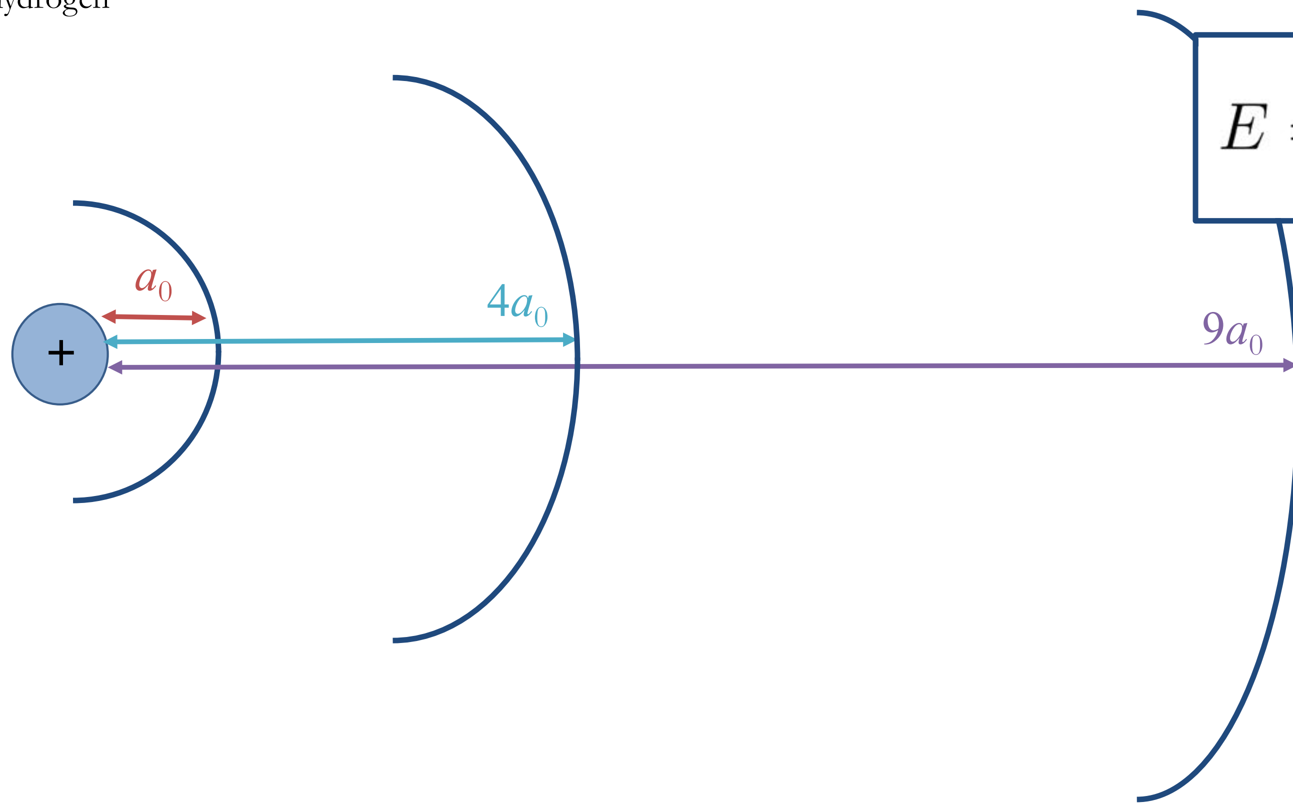
Atomic Structure and Spectral Lines



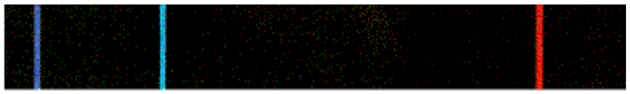
Emission lines of the "Balmer series" of hydrogen

Recall that one of the great successes of Bohr's (1913) model of the atom was that it could account for the *spectral lines* of hydrogen, such as the Balmer series.

$$E = -\frac{1}{2}\frac{me^4}{\hbar^2}\frac{1}{n^2}$$



Atomic Structure and Spectral Lines



Emission lines of the "Balmer series" of hydrogen

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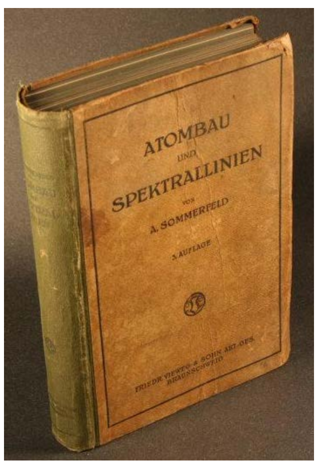
By the 1890s, physicists had observed *splittings* in such spectral lines, when the gas was placed in an *external magnetic field*: a single sharp line (when $\mathbf{B} = 0$) would appear as a closely-spaced *triplet* of lines (when $\mathbf{B} \neq 0$): the "Zeeman effect."

Emission line, no external **B** field

Emission lines in the presence of an external **B** field

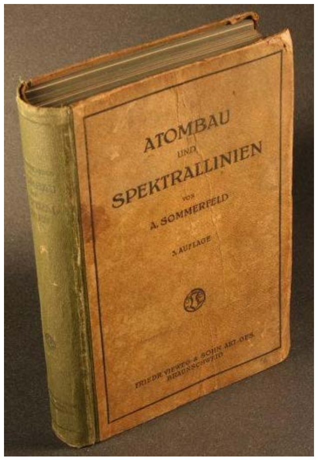


1st edition: 1919

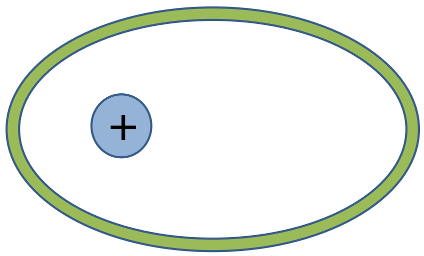
Arnold Sommerfeld, the Ordinarius Professor of theoretical physics in Munich, worked with his graduate students* to understand the puzzles of "atomic structure and spectral lines." They began by *generalizing* Bohr's model to *elliptical orbits*.

* *Werner Heisenberg*, *Wolfgang Pauli*, *Hans Bethe*, ...

Sommerfeld's Approach



For simplicity, Bohr had considered circular orbits of electrons in simple atoms like hydrogen. But (just as in celestial mechanics), Sommerfeld argued that the most general motion should be *ellipses*.



$$E = \frac{p_r^2}{2m} + \frac{L^2}{2r^2} - \frac{e^2}{r}$$

(L: angular momentum)

Whereas a circular orbit has only *one* degree of freedom (r), an elliptical orbit has *two* degrees of freedom (r and φ). So Sommerfeld proposed a *generalization* of Bohr's "quantum condition." *Each* degree of freedom should be subject to quantization:

$$\oint p_r \, dr = n_r h$$

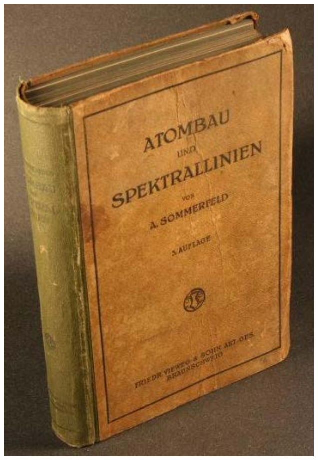
$$\oint L \, d\varphi = n_\varphi h$$

$$E = -\frac{me^4}{2\hbar^2 \left(n_r + n_\varphi\right)^2}$$

(Same as Bohr's expression, but with $n \rightarrow n_r + n_\varphi$)

$$n_r \geq 1 \,, \; 0 \leq n_\varphi \leq n_r \text{ -1}$$

Sommerfeld's Approach



If one *quantizes* the orbital angular momentum **L** (in units of $\hbar$), then the *projection* of **L** along a given direction **z** will only take discrete values, $m_l \hbar = \mathbf{L} \cdot \mathbf{z}$, with

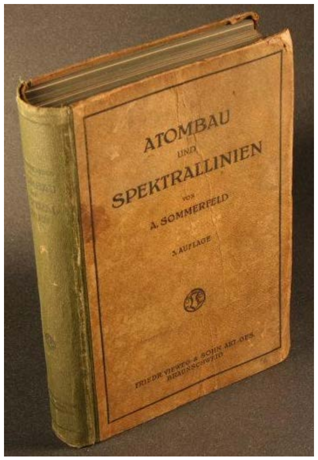
$$- n_\varphi \leq m_l \leq n_\varphi .$$

For $n_\varphi = 1$, $m_l \in \{-1, 0, +1\}$; for $n_\varphi = 2$, $m_l \in \{-2, -1, 0, +1, +2\}$. For any integer n_φ, there will be $(2 n_\varphi + 1)$ values of m_l: *always an odd number.*

So now in place of only *one* quantum number, as in Bohr's model, Sommerfeld and his students began considering *three* quantum numbers: (n_r, n_φ, m_l), each of which could only take on integer values.

Note Sommerfeld's strategy: much like other work within "old quantum theory," he began with *classical* descriptions of objects' motion, and then appended special "quantum conditions" to constrain the allowable motion.

Sommerfeld’s Approach



Why would anyone pursue such baroque complexity? Because Sommerfeld quickly found a way to address Zeeman’s observed splitting of spectral lines into triplets.

Emission line, no external **B** field

Emission lines in the presence of an external **B** field

An electric charge q that is moving with some angular momentum **L** will have a *magnetic moment*

$$\boldsymbol{\mu} = \frac{q}{2m}\mathbf{L}$$

In an external magnetic field, the energy of the system will depend on the relative orientation of $\boldsymbol{\mu}$ and **B**:

$$\Delta E = -\boldsymbol{\mu} \cdot \mathbf{B}$$

If one quantized **L** (and hence $\boldsymbol{\mu}$), the energy levels of an electron *in an external magnetic field* would be *split* into m_l distinct levels. The Zeeman triplets must have come from electrons making transitions from an orbit with $n_\varphi = 1$ (and hence m_l = -1, 0, +1) to an orbit with $n_\varphi = 0$ (and hence $m_l = 0$). The light emitted from those transitions would have *slightly different energies*, yielding the three closely-spaced spectral lines.

“Anomalous” Zeeman Effect

Sommerfeld’s approach — treat an electron’s motion with all the tools of classical mechanics, then impose “quantum conditions” to restrict values of certain quantities — addressed the “ordinary” Zeeman splitting into triplets. But there was also evidence of an “anomalous” Zeeman effect: *doublets!*

Emission line, no external **B** field

Emission lines in the presence of an external **B** field

One of Sommerfeld’s students, *Wolfgang Pauli*, worked on the challenge while a postdoc with Niels Bohr in Copenhagen in the early 1920s.

“A colleague who met me strolling rather aimlessly in the beautiful streets of Copenhagen said to me in a friendly manner, ‘You look very unhappy’; whereupon I answered fiercely, ‘How can one look happy when he is thinking about the anomalous Zeeman effect?’ ” – Pauli recollections

Copenhagen ca. 1900

"Anomalous" Zeeman Effect

Graduate students of Hendrik Lorentz in Leiden, *George Uhlenbeck* and *Samuel Goudsmit*, were also working on the anomalous Zeeman effect.

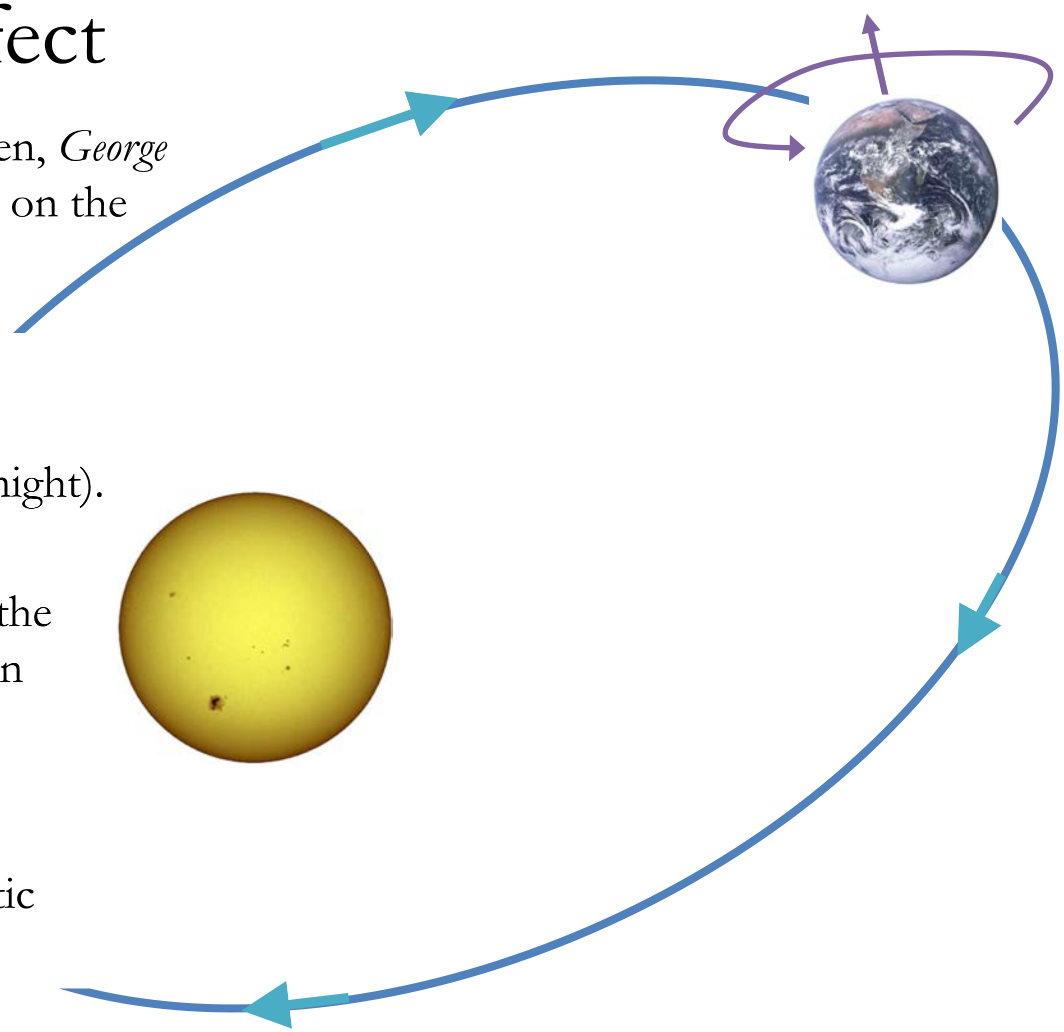
They reasoned that the *Earth* has *two* kinds of angular momentum: it orbits the Sun (Keplerian elliptical orbit), *and* it spins on its own axis (day/night).

If the electron had an *intrinsic* "spin" **S** (akin to the Earth's rotation around its own axis), *and* that spin were *quantized,*

$$|\mathbf{S}| = \frac{1}{2}\hbar$$

then the electron would have an *additional* magnetic moment:

$$\boldsymbol{\mu}_s = \frac{q}{2m}\boldsymbol{S}$$



“Anomalous” Zeeman Effect

Emission line, no external **B** field

Emission lines in the presence of an external **B** field

Goudsmit and Uhlenbeck then argued as Sommerfeld had done: in an external **B** field, $\Delta E = -\boldsymbol{\mu}_s \cdot \mathbf{B}$. *If* the “spin” could only ever line up *parallel* or *antiparallel* to **B**, then there should be *doublets* of various spectral lines, whose separation depended on $|\mathbf{S}| = \hbar/2$. They called this “*space quantization*”: the spin vector could only point along *discrete* directions in space.

By fixing the magnitude $|\mathbf{S}| = \hbar/2$, they found a close match to Zeeman’s results. But with a (conceptual) price: with that magnitude of $|\mathbf{S}|$, a point on the electron’s equator would be spinning *faster than the speed of light*, and its *mass* would *diverge*. By 1924, such a value of spin — if imagined as a real, physical motion — seemed absurd; the effect seemed impossible to *visualize*.

Their advisor, Lorentz, cautioned them not to publish. But their *other* advisor, *Paul Ehrenfest*, had already sent their paper to a journal without telling them! “You’re still young enough to afford a stupidity,” he explained.*

*By today’s standards, Ehrenfest’s actions were totally unethical. Advisors today would put *their own name* on the paper and *then* submit it to a journal, behind their students’ backs...

“Anomalous” Zeeman Effect

Copenhagen ca. 1900

Independent of Goudsmit and Uhlenbeck, Wolfgang Pauli introduced his “exclusion principle” early in 1925.

Following his own advisor, Arnold Sommerfeld, Pauli considered adding a *fourth* quantum number, n_s, which (like the other n_i) could only take on certain discrete values.

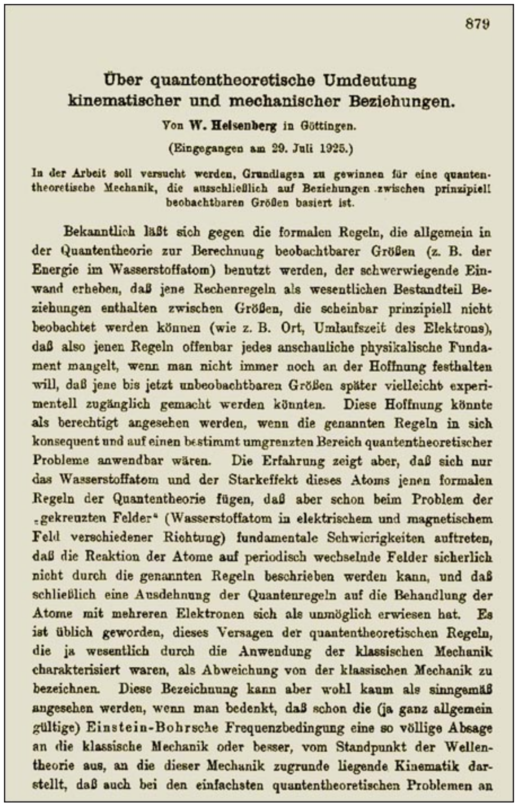
He argued that if this fourth quantum number had a “*classically indescribable double-valuedness*” (i.e., could only take on 2 values), then one could account for the anomalous Zeeman effect as well as other features of atomic structure.

This became known as the *Pauli exclusion principle*: electrons in an atom must be described by four quantum numbers (n_r, n_φ, m_l, n_s), and no two electrons can have the same set of quantum numbers at the same time.

Pauli later claimed to have been inspired by the precision of *Can-Can* dancers, who always managed to get out of each other’s spot at the last moment.

Questions?

Heisenberg and Matrix Mechanics



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Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen.

Von **W. Heisenberg** in Göttingen.

(Eingegangen am 29. Juli 1925.)

In der Arbeit soll versucht werden, Grundlagen zu gewinnen für eine quantentheoretische Mechanik, die ausschließlich auf Beziehungen zwischen prinzipiell beobachtbaren Größen basiert ist.

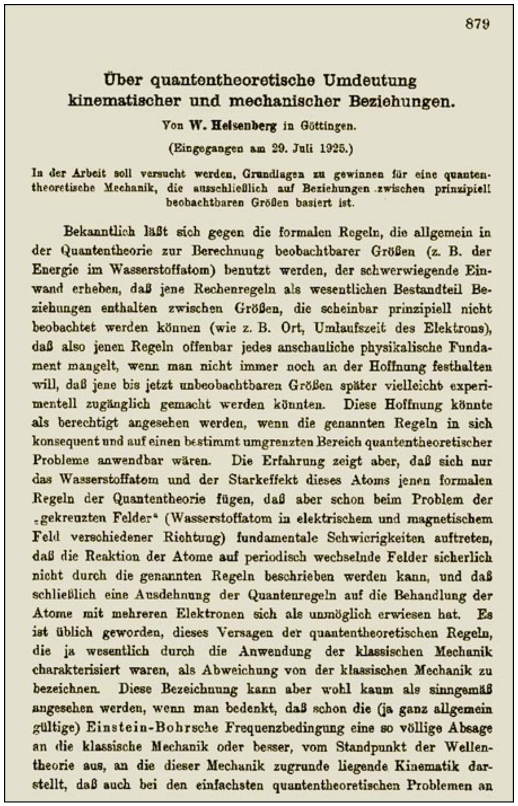
Bekanntlich läßt sich gegen die formalen Regeln, die allgemein in der Quantentheorie zur Berechnung beobachtbarer Größen (z. B. der Energie im Wasserstoffatom) benutzt werden, der schwerwiegende Einwand erheben, daß jene Rechenregeln als wesentlichen Bestandteil Beziehungen enthalten zwischen Größen, die scheinbar prinzipiell nicht beobachtet werden können (wie z. B. Ort, Umlaufszeit des Elektrons), daß also jenen Regeln offenbar jedes anschauliche physikalische Fundament mangelt, wenn man nicht immer noch an der Hoffnung festhalten will, daß jene bis jetzt unbeobachtbaren Größen später vielleicht experimentell zugänglich gemacht werden könnten. Diese Hoffnung könnte als berechtigt angesehen werden, wenn die genannten Regeln in sich konsequent und auf einen bestimmt umgrenzten Bereich quantentheoretischer Probleme anwendbar wären. Die Erfahrung zeigt aber, daß sich nur das Wasserstoffatom und der Starkeffekt dieses Atoms jenen formalen Regeln der Quantentheorie fügen, daß aber schon beim Problem der „gekreuzten Felder“ (Wasserstoffatom in elektrischem und magnetischem Feld verschiedener Richtung) fundamentale Schwierigkeiten auftreten, daß die Reaktion der Atome auf periodisch wechselnde Felder sicherlich nicht durch die genannten Regeln beschrieben werden kann, und daß schließlich eine Ausdehnung der Quantenregeln auf die Behandlung der Atome mit mehreren Elektronen sich als unmöglich erwiesen hat. Es ist üblich geworden, dieses Versagen der quantentheoretischen Regeln, die ja wesentlich durch die Anwendung der klassischen Mechanik charakterisiert waren, als Abweichung von der klassischen Mechanik zu bezeichnen. Diese Bezeichnung kann aber wohl kaum als sinngemäß angesehen werden, wenn man bedenkt, daß schon die (ja ganz allgemein gültige) Einstein-Bohrsche Frequenzbedingung eine so völlige Absage an die klassische Mechanik oder besser, vom Standpunkt der Wellentheorie aus, an die dieser Mechanik zugrunde liegende Kinematik darstellt, daß auch bei den einfachsten quantentheoretischen Problemen an

Heisenberg, "On the quantum-theoretical reinterpretation of kinematic and mechanical relationships," 1925

One of Pauli's close friends, *Werner Heisenberg* — another recent PhD student of Sommerfeld's — shared Pauli's frustration with the approach of trying to find visualizable, classical models and then appending ad hoc "quantum conditions." In 1924, Heisenberg began a postdoc position with Niels Bohr in Copenhagen.

Heisenberg sought a new "*quantum mechanics*": a first-principles treatment of the atomic realm, rather than a kludge. He sought to break the impasse of the Bohr-Sommerfeld approach by returning to Einstein's (Machian) positivism of 1905: we can never *observe* an electron in its orbit within an atom, so we should stop trying to calculate atomic properties on the basis of quasi-classical orbits.

Heisenberg and Matrix Mechanics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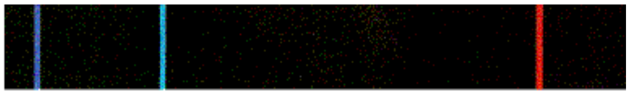
“It seems sensible to discard all hope of observing hitherto unobservable quantities [like an electron’s orbit]. Instead it seems more reasonable to try to establish a theoretical quantum mechanics, analogous to classical mechanics, but in which only relations between *observable quantities* appear. [... Previous approaches could be] seriously criticized on the grounds that they contain, as basic elements, relationships between quantities that are apparently *unobservable in principle*, such as position and period of revolution of the electron.”

Einstein’s response: “A good joke shouldn’t be repeated too often.”

Heisenberg and Matrix Mechanics



Emission lines of the "Balmer series" of hydrogen

Heisenberg argued that physicists should focus on *empirical quantities*, such as the frequencies of spectral lines. In particular, the frequencies of spectral lines obeyed a *law of addition*.

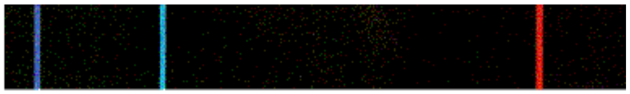
$$\nu_{nm} = R\left[\frac{1}{n^2} - \frac{1}{m^2}\right]$$

$$\begin{aligned}\nu_{nk} + \nu_{km} &= R\left[\frac{1}{n^2} - \frac{1}{k^2} + \frac{1}{k^2} - \frac{1}{m^2}\right] \\ &= R\left[\frac{1}{n^2} - \frac{1}{m^2}\right] \\ &= \nu_{nm}\end{aligned}$$

This relationship could be extended: $\nu_{nm} = \nu_{nk} + \nu_{kj} + \nu_{jm}$. In other words, an electron could jump from (say) $m = 6$ to $n = 1$ all at once (ν_{16}), or via $6 \rightarrow 3$, $3 \rightarrow 1$, or $6 \rightarrow 3$, $3 \rightarrow 2$, $2 \rightarrow 1$, and so on.

Heisenberg began to consider *arrays* of these *observable quantities*, ν_{nm}.

Heisenberg and Matrix Mechanics



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Island of Heligoland, off the coast of Denmark

$$\nu_{nk} + \nu_{km} = R\left[\frac{1}{n^2} - \frac{1}{k^2} + \frac{1}{k^2} - \frac{1}{m^2}\right]$$
$$= R\left[\frac{1}{n^2} - \frac{1}{m^2}\right]$$
$$= \nu_{nm}$$

In May 1925, in the midst of these studies, Heisenberg suffered from hay fever and traveled to the island of *Heligoland* in the North Sea. There he continued his work for about two weeks.

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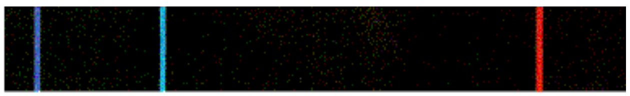
Heisenberg and Matrix Mechanics



Emission lines of the "Balmer series" of hydrogen

On the island, Heisenberg reasoned: these frequencies ν refer to spectral lines, that is, to *light*, so they appear in the *exponent* when describing light waves:

frequency

$$E = A\, e^{2\pi i \nu t}$$

amplitude

If the frequencies ν *add*, then the amplitudes A must *multiply:*

$$(a \times 10^{x}) \times (b \times 10^{y}) = (a \times b) \times 10^{x+y}$$

So if $\nu_{nm} = \nu_{nk} + \nu_{km}$, one should require $A_{nm} = (A_{nk}) \times (A_{km})$. *But* Heisenberg found:

$$A_{nk} \times A_{km} \neq A_{km} \times A_{nk}$$

The *order of multiplication* changed the result!

Heisenberg and Matrix Mechanics

Göttingen Institute for Theoretical Physics

Soon after finishing his paper, Heisenberg began a new position in Göttingen, working closely with the mathematical physicist *Max Born*. Born's reaction: "You dummkopf! You're studying *matrices*!"*

$$A = \begin{pmatrix} 1 & 2 \\ 1 & 2 \end{pmatrix}, \; B = \begin{pmatrix} 0 & 3 \\ 1 & 0 \end{pmatrix}$$

$$A \times B = \begin{pmatrix} 1 & 2 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} 0 & 3 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 3 \\ 2 & 3 \end{pmatrix}$$

$$B \times A = \begin{pmatrix} 0 & 3 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 2 \\ 1 & 2 \end{pmatrix} = \begin{pmatrix} 3 & 6 \\ 1 & 2 \end{pmatrix}$$

The fact that $A \times B \neq B \times A$ is a *general feature* of matrix multiplication: *matrices do not commute.*

*a rough paraphrase...

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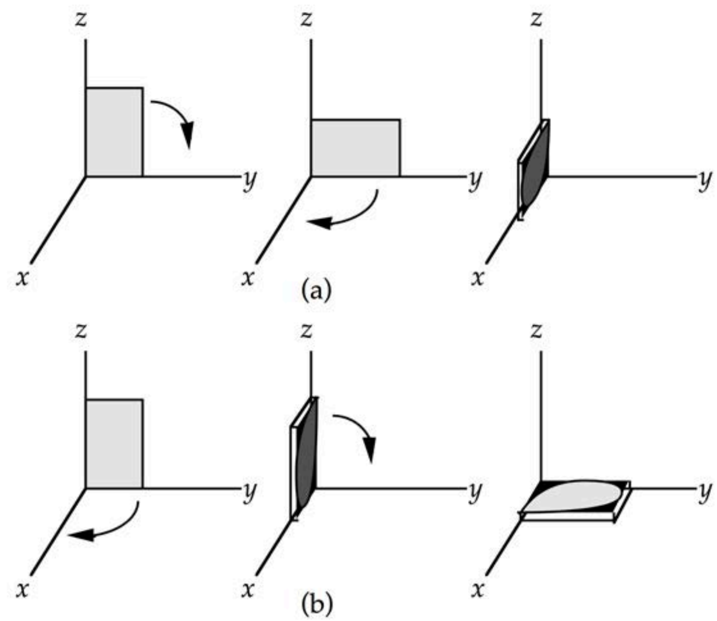

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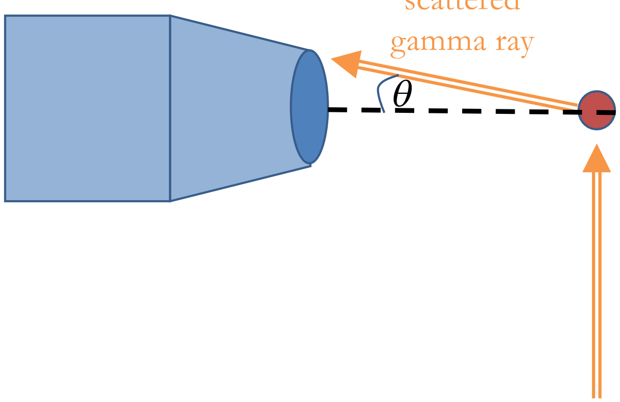
Questions?

The Uncertainty Principle

Niels Bohr's Institute, Copenhagen

In Heisenberg's formulation, physical quantities are represented by *matrices*; hence the *outcome* of transformations depends on the *order* of operations.

In the spring of 1927, Heisenberg returned to Bohr's Institute in Copenhagen. He aimed to work out a *physical interpretation* of what non-commuting matrices might mean for the quantum realm. He imagined a *gamma-ray microscope*.



If we want to measure the *position* of an electron, we can bounce light off of it and collect the scattered light. But the electron is *small*, so we need light with a *small wavelength* λ (large frequency) to get good resolution.

Any light scattered within an angle θ will enter the aperture of the microscope. *Resolving power*:

$$\delta x = \frac{\lambda}{\sin\theta}$$

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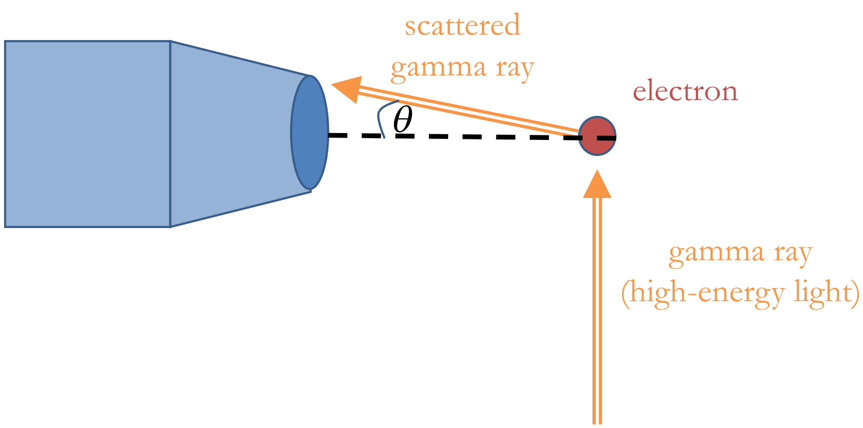
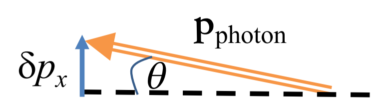


The aperture will collect scattered light with momenta $\mathbf{p}_{\text{photon}}$ within a cone of angular size θ: the scattered photons could have *any* component p_x within $\delta p_x = |\mathbf{p}_{\text{photon}}| \sin\theta$.



Following the scattering, the *electron* will acquire some momentum within $\delta p_x = |\mathbf{p}_{\text{photon}}| \sin\theta$.

But $|\mathbf{p}_{\text{photon}}| = h/\lambda$.

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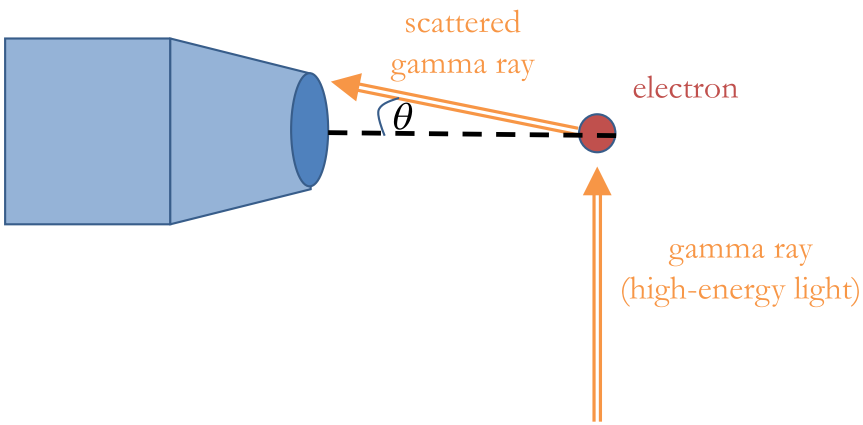

Combine:

$$\delta x\, \delta p_x \sim \left(\frac{\lambda}{\sin\theta}\right)\left(\frac{h}{\lambda}\sin\theta\right) = h \neq 0$$

One cannot make *both* δx *and* δp_x arbitrarily small at the same time!

The Uncertainty Principle

Niels Bohr's Institute, Copenhagen

$$\delta x \, \delta p_x \sim h$$

Heisenberg intrepreted this result as a *disturbance*: we are clumsy, and we can't help but disturb tiny things like electrons when we try to measure their properties.

Bohr strongly disagreed. During intense — sometimes tear-streaked — discussions throughout the spring and summer of 1927, Heisenberg and Bohr argued over how to make sense of the new *uncertainty principle*.*

Bohr's interpretation: $\delta x \, \delta p_x \sim h$ is *not* a result of our clumsiness, but a fact about *quantum objects themselves*: they simply do not and cannot have simultaneously sharp values for certain pairs of properties. To Bohr, the electron did *not* have $\delta x \, \delta p_x = 0$, even *before* it was smacked by the photon.

* See Megan Shields Formato reading: Bohr was *always* working in dialogue with other people, most often his wife *Margrethe Bohr* (who rarely received any credit). Sometimes these dialogues became quite emotional!

The Uncertainty Principle

Niels Bohr's Institute, Copenhagen

$$\delta x \, \delta p_x \sim h$$

If the uncertainty principle held for quantum objects themselves (and not just as a consequence of our interactions with them), then there could be *no trajectories* for quantum objects: after all, a trajectory requires knowing *where an object is* and *where it is going* at each moment in time.

To Bohr, at least, the uncertainty principle seemed to imply that given $x(t_0)$, one *cannot* know $x(t_1)$ with certainty. This suggested the *fall of determinism*: given the present state of a system and knowledge of the forces acting on it was *no longer sufficient* to predict with certainty what would happen in the future.

Bohr eventually convinced Heisenberg of this broader conception; Bohr came to call it "the general epistemological lesson of the quantum."