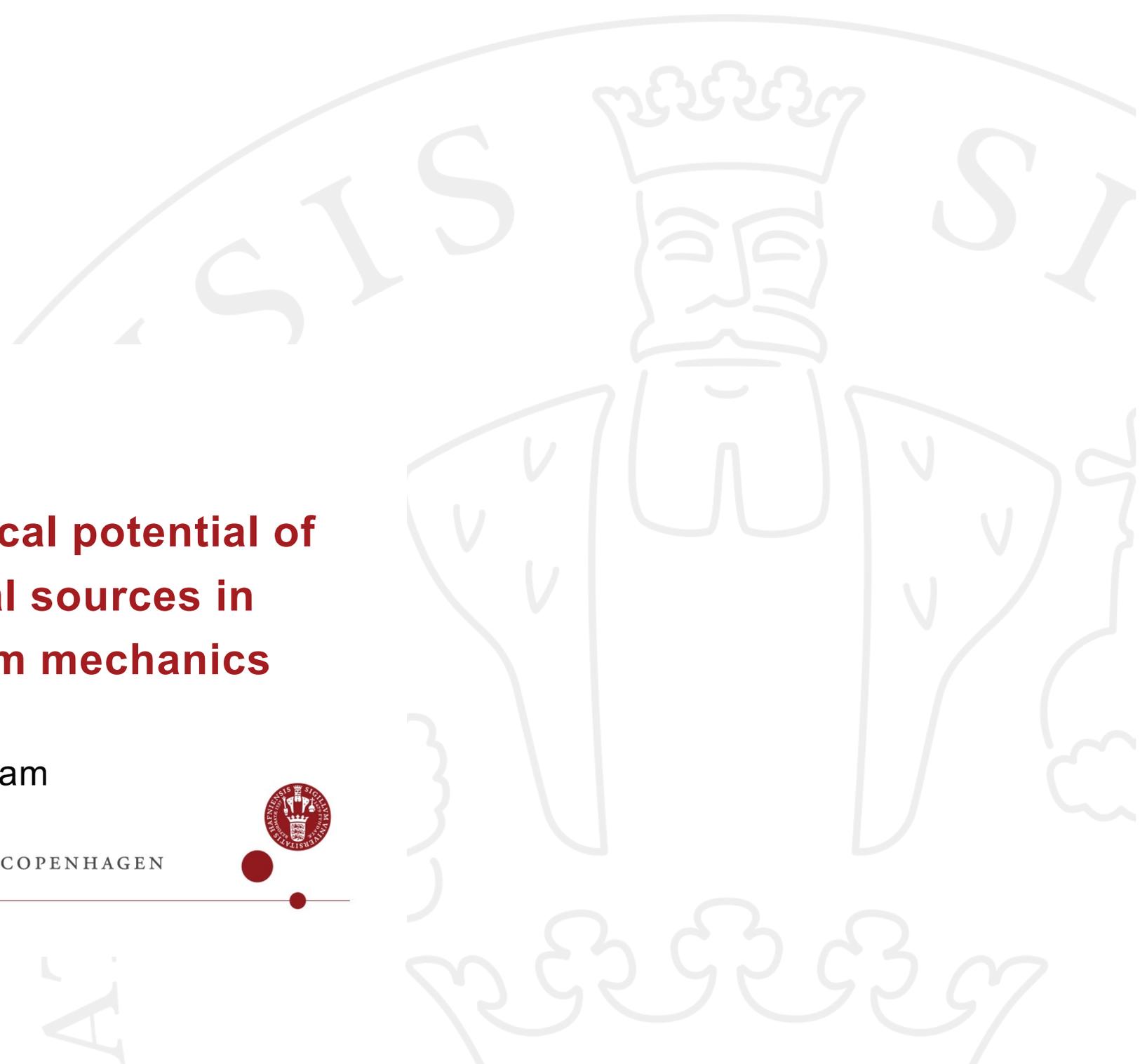


Pedagogical potential of original sources in quantum mechanics

Ricardo Karam

UNIVERSITY OF COPENHAGEN



QM teaching is usually dogmatic and pragmatic

Postulate 1

At any times the state of a **physical system is represented by a state vector** $|\psi\rangle$ which is an element of **Hilbert space** \mathcal{H} .

Postulate 2

An **observable** A of a physical system is described by a **linear Hermitian operator** \hat{A} that acts in \mathcal{H} .

Postulate 3

The only possible **result of the measurement** of an observable A is one of the **eigenvalues** a_n of the corresponding operator \hat{A} .

Postulate 4

When a measurement of an observable A is made on a normalized state $|\psi\rangle$ the **probability of obtaining an eigenvalue** a_n with degeneracy d_n is

$$P_n = \sum_{i=1}^{d_n} |c_n^{(i)}|^2 \text{ with } c_n^{(i)} \equiv \langle a_n^{(i)} | \psi \rangle.$$

Postulate 5

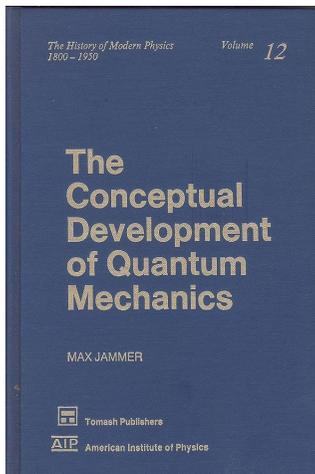
Immediately **after the measurement** of an observable A has yielded a value a_n the state of the **system is in the eigenstate**

$$|\psi\rangle = \frac{1}{\sqrt{P_n}} \sum_{i=1}^{d_n} c_n^{(i)} |a_n^{(i)}\rangle.$$

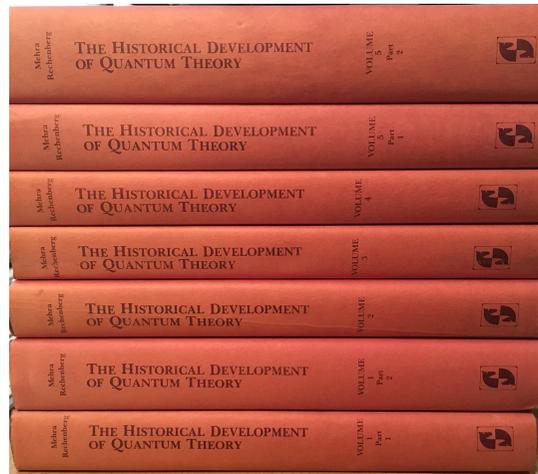


<https://www.amazon.com/Funny-Quantum-Physics-Calculate-T-Shirt/dp/B07VFWGCWQ>

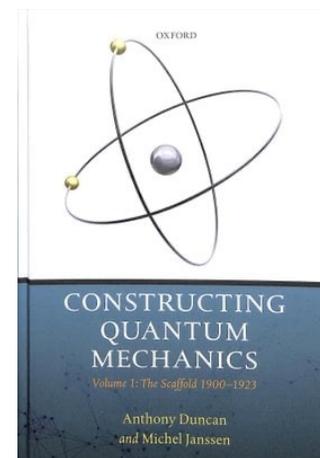
Dogmatic/Pragmatic for good reasons: History is super complicated!



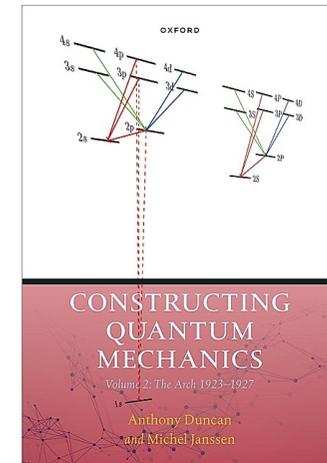
Max Jammer



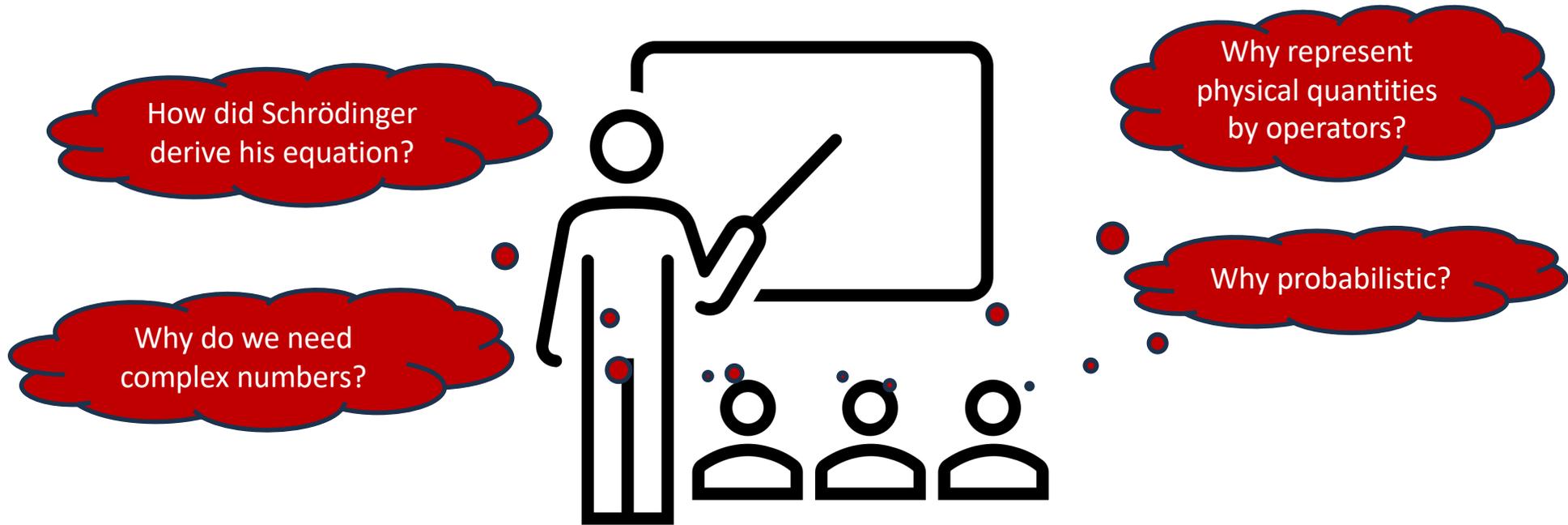
Mehra & Rechenberg



Duncan & Janssen



But from the learner's perspective, this can be frustrating

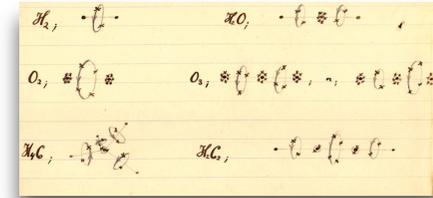


Can we find a compromise? Didactical design!

- Careful selection: short (3-page!) excerpts, deep insights
- Clear learning goals; Good secondary sources
- *A posteriori*: Comparison with modern teaching

Selected Episodes: A glimpse of how...

1) Bohr first proposed his **model**



2) Heisenberg introduced **matrices** to the QM formalism

Über quantentheoretische Umdeutung
kinematischer und mechanischer Beziehungen.

Von W. Heisenberg in Göttingen.

(Eingegangen am 29. Juli 1925.)

3) Schrödinger **derived** his equation and interpreted the real part of ψ

Four Lectures on
Wave Mechanics

Delivered at the Royal Institution, London, on
5th, 7th, 12th, and 14th March, 1928

4) Born arrived at his **statistical interpretation**

Zur Quantenmechanik der Stoßvorgänge.

[Vorläufige Mitteilung.¹]

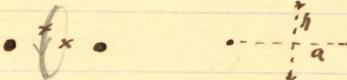
Von **Max Born**, Göttingen.

(Eingegangen am 25. Juni 1926.)

Rutherford (aka Manchester) memorandum 1912

Hydrogen

[H]  Central force = $\frac{e^2}{r^2} \cdot 1$

H_2  $\frac{e^2}{4a^2} = 2 \cdot \frac{e^2 \cdot a}{(a^2 + h^2)^{3/2}} \quad h = a\sqrt{3}$

Central force = $2 \cdot \frac{e^2 \cdot h}{(a^2 + h^2)^{3/2}} = \frac{e^2}{4h^2} = \frac{e^2}{h^2} \left(\frac{3\sqrt{3}}{4} - \frac{1}{4} \right) = \frac{e^2}{h^2} \cdot 1.049$

Helium

He  Central force $\frac{2e^2}{r^2} = \frac{e^2}{4h^2} = \frac{e^2}{h^2} \cdot 1.75$

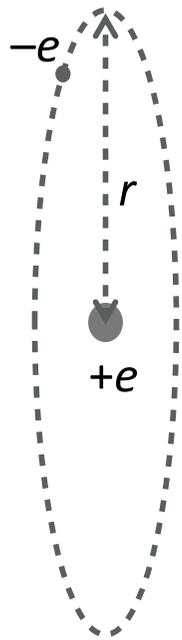
[He₂]  $\frac{4e^2}{4a^2} = 4 \cdot \frac{2e^2 \cdot a}{(a^2 + h^2)^{3/2}} \quad h = a\sqrt{3}$

Central force = $2 \cdot \frac{2e^2 \cdot h}{(a^2 + h^2)^{3/2}} = \frac{e^2 \cdot A_v}{4h^2} = \frac{e^2}{h^2} \left(\frac{3\sqrt{3}}{2} - \frac{3.828}{4} \right) = \frac{e^2}{h^2} \cdot 1.641$

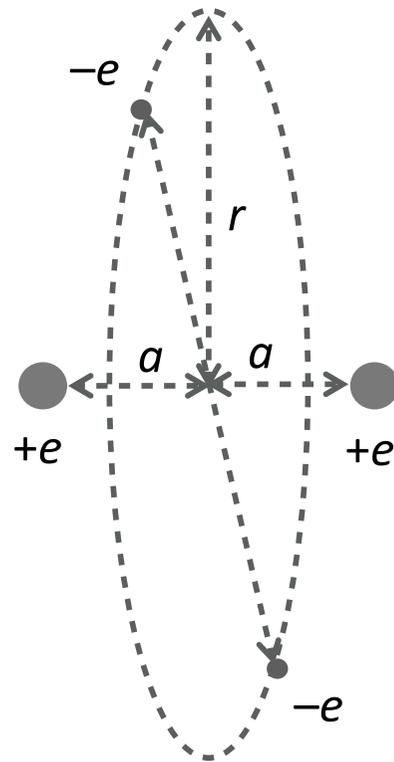
If we put the force equal to $\frac{e^2 \cdot X}{h^2}$ we get

[H]	H_2	He	[He ₂]
1	1.049	1.75	1.641

Stability and formation of H_2 and He_2



hydrogen atom



hydrogen molecule

hydrogen atom

Centripetal force = Coulomb force

$$m\omega^2 r = \frac{e^2}{r^2} \longrightarrow m\omega^2 r^3 = e^2$$

hydrogen molecule

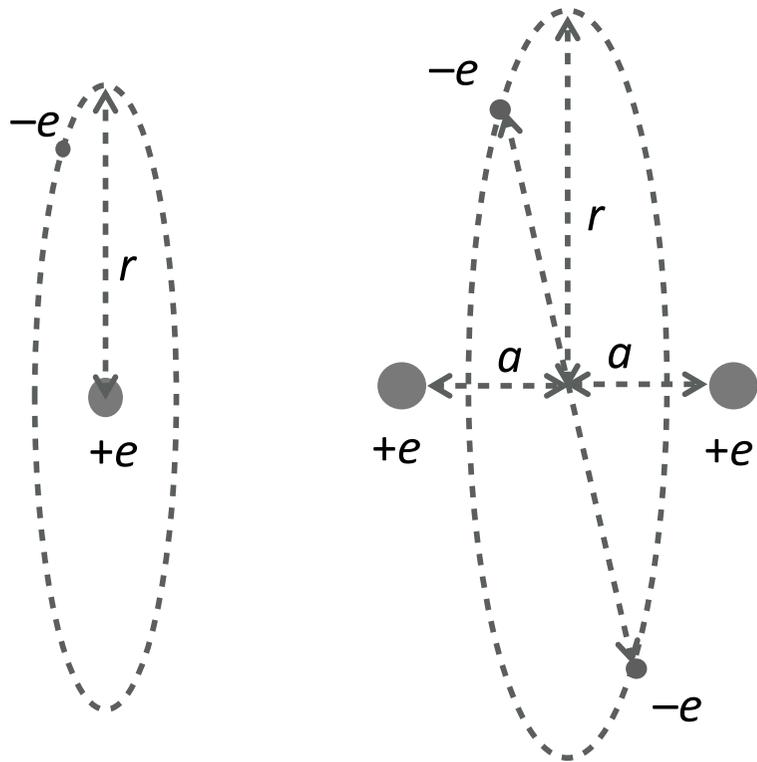
Condition for nuclear stability

$$\frac{e^2}{4a^2} = 2 \cdot \frac{e^2}{a^2+r^2} \cdot \frac{a}{\sqrt{a^2+r^2}} = \frac{2e^2 a}{(a^2+r^2)^{3/2}}$$

$$(a^2+r^2)^{3/2} = 8a^3 \longrightarrow a^2 + r^2 = 8^{2/3} a^2 = 4a^2$$

$$a^2 = r^2/3 \quad r = a\sqrt{3}$$

Stability and formation of H_2 and He_2



hydrogen atom

hydrogen molecule

Similar procedure to Helium

hydrogen atom

Centripetal force = Coulomb force

$$m\omega^2 r = \frac{e^2}{r^2} \rightarrow m\omega^2 r^3 = e^2$$

hydrogen molecule

Centripetal force

(per electron)

$$m\omega^2 r = 2 \cdot \frac{e^2}{a^2 + r^2} \cdot \frac{r}{\sqrt{a^2 + r^2}} - \frac{e^2}{4r^2}$$

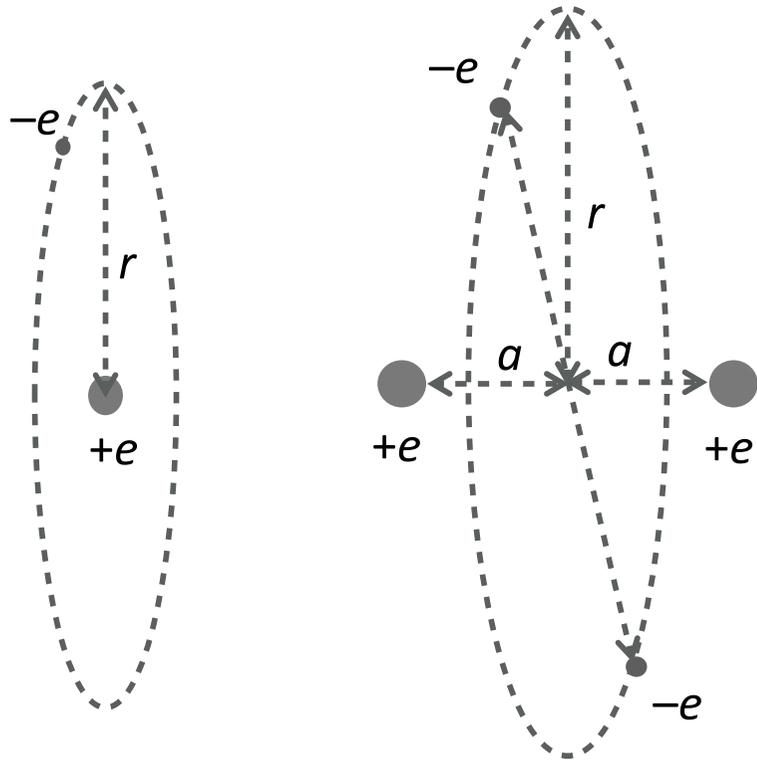
$$m\omega^2 r = X \cdot \frac{e^2}{r^2} \text{ with } X = \frac{3\sqrt{3}-1}{4} \cong 1.049$$

Central force = $2 \cdot \frac{e^2 \hbar}{(a^2 + \hbar^2)^{3/2}} - \frac{e^2}{4r^2} = \frac{e^2}{\hbar^2} \left(\frac{3\sqrt{3}}{4} - \frac{1}{4} \right) = \frac{e^2}{\hbar^2} \cdot 1.049$

If we put the force equal to $\frac{e^2 X}{r^2}$ we get

[H]	H ₂	He	[He ₂]
1	1.049	1.75	1.641

Planck's constant enters Bohr's model



hydrogen atom

hydrogen molecule

In general $m\omega^2 r^3 = Xe^2$

Hydrogen atom: $X = 1$

Hydrogen molecule: $X = 1.049$

How to fix ω and r ?

$$E_{kin} = K\nu \quad \frac{1}{2} m\omega^2 r^2 = K \frac{\omega}{2\pi}$$

$$m\omega r^2 = \frac{K}{\pi}$$

$$m\omega^2 r^4 = \frac{K^2}{m\pi^2}$$

$$r = \frac{K^2}{\pi^2 X m e^2}$$

$$\omega = \frac{m\pi^3 e^4 X^2}{K^3} \quad \nu = \frac{m\pi^2 e^4 X^2}{2K^3}$$

Pause for reflection...

- Is there anything being quantized?
- Where are the spectral lines?
- What is the value of Planck's constant?
- Are there quantum jumps?

The pivoting role of Balmer's formula

- **Hans Marius Hansen (1886–1956)** points out Balmer's formula to Bohr

$$\nu = R \left(\frac{1}{n^2} - \frac{1}{m^2} \right),$$

where n and m are integers such that $m > n$ and R is the Rydberg constant.

- Bohr later said: "as soon as I saw Balmer's formula, the **whole thing was immediately clear** to me."

The royal road from the Memorandum to Balmer's formula

- Total energy of an electron in Bohr's model of the hydrogen atom: $E_{\text{tot}} = -\frac{\pi^2 m e^4}{2K^2}$
- "Quantization" condition: $E_{\text{kin}} = K\nu$. Comparison with the quantization condition for a Planck oscillator, $E_{\text{tot}} = \tau h\nu$, which means that $E_{\text{kin}} = \frac{1}{2}\tau h\nu$, suggests that we set $K = \frac{1}{2}\tau h$ (for $\tau = 1$, $K = .5h$).
- Hence $E_{\text{tot}} = -\frac{2\pi^2 m e^4}{\tau^2 h^2}$
- We get the Balmer formula if we make the *now familiar assumption* that the **energy lost when an electron jumps** from an energy state labeled by τ_1 to an energy state labeled by $\tau_2 < \tau_1$ is emitted as radiation with a frequency ν equal to this energy loss divided by Planck's constant:

$$\nu = \frac{E_{\text{tot}}^{(\tau_1)} - E_{\text{tot}}^{(\tau_2)}}{h} = \frac{2\pi^2 m e^4}{h^3} \left(\frac{1}{\tau_2^2} - \frac{1}{\tau_1^2} \right)$$

$$\nu = R \left(\frac{1}{n^2} - \frac{1}{m^2} \right),$$

Problems to explain the $\frac{1}{2}$ factor

- Bohr's initial justification of the quantum condition $K = \frac{1}{2} \tau h$
 - ~ Radiation is emitted when an electron is captured by a nucleus and settles into an orbit with energy $E_{\text{tot}} = -\tau h \omega / 2$. The energy lost by the electron is emitted in τ quanta of energy as monochromatic radiation (in the form of waves) of frequency $\omega/2$, the average between the electron's initial frequency (0) and its final frequency (ω).
 - ~ The real reason for this factor $\frac{1}{2}$: Bohr knew he needed it to get the right value for the Rydberg constant ...

- Problems with Bohr's initial proposal:
 - ~ The 'emission-following-electron-capture' radiation mechanism (pp. 4–5) needs to be replaced by an 'emission-following-transition-between-states' mechanism (p. 7) to get the Balmer formula. **This replacement comes at the price of severing the relation between orbital frequencies and radiation frequencies!**

A controversial step



Thomas S. Kuhn (1922–1996)

Heilbron and Kuhn 1969: "That a spectral line of a given frequency must be produced by a charge vibrating at the same frequency was a consequence of electromagnetic theory which **even Planck and Einstein had not thought to challenge.**"

Schrödinger to Lorentz, June 6, 1926: "The frequency discrepancy in the Bohr model ... seems to me, (and has indeed seemed to me since 1914), to be something *so monstrous*, that I should like to characterize the excitation of light in this way as really almost *inconceivable*"

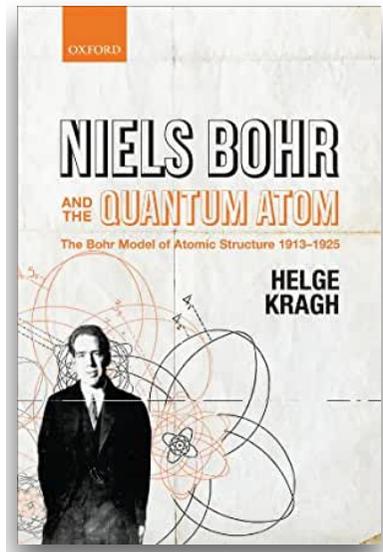


Erwin Schrödinger (1887–1961)

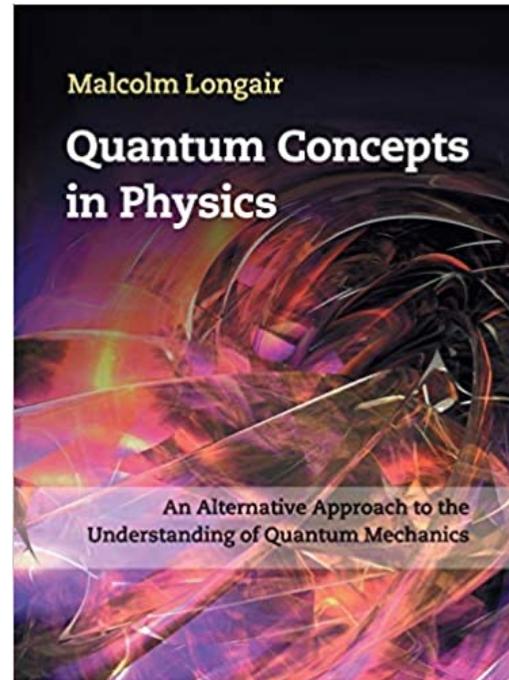
Useful references

The Genesis of the Bohr Atom

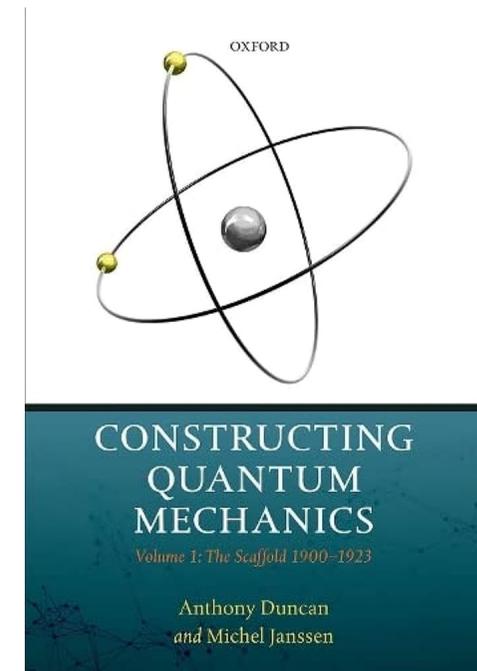
BY JOHN L. HEILBRON* AND THOMAS S. KUHN**



Historical research



Didactic reconstruction



Some lessons from case 1)

- At first, Bohr was **not** interested in explaining the hydrogen spectrum (otherwise considered his key achievement); he was way **more ambitious** than textbooks would have him appear (explain **all molecules**).
- The (in)famous electron jumps were inferred from the structure of Balmer's formula;
- Bohr had problems explaining a $\frac{1}{2}$ factor theoretically, although its need was clear from the experimental value of R
- Orbital frequency \neq radiation frequency: MAJOR controversy!

The quantum century (2025)

Heisenberg's breakthrough in Helgoland

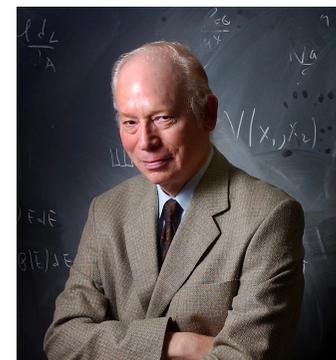


Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen.

Von W. Heisenberg in Göttingen.

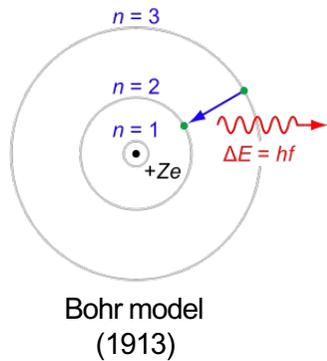
(Eingegangen am 29. Juli 1925.)

On the quantum-theoretical reinterpretation of kinematic and mechanical relationships



I have never understood Heisenberg's motivations for the mathematical steps in his paper (Steven Weinberg)

The Correspondence Principle (TCP)

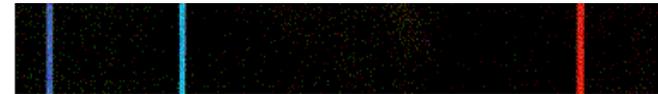


The electron motion is **no longer the cause** of radiation
Says **nothing** about the **intensity** of the radiation

Quantum jumps and classical harmonics

American Journal of Physics 70, 332 (2002); <https://doi.org/10.1119/1.1445405>

William A. Fedak and Jeffrey J. Prentis



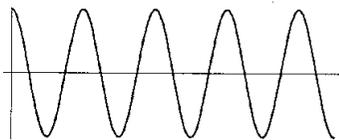
Emission lines of hydrogen

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

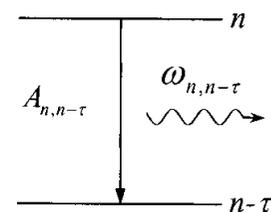
5 → 4	ω'	500 → 499	ω
5 → 3	$3.2\omega'$	500 → 498	2.0ω
5 → 2	$9.3\omega'$	500 → 497	3.0ω
5 → 1	$43\omega'$	500 → 496	4.0ω

Classical

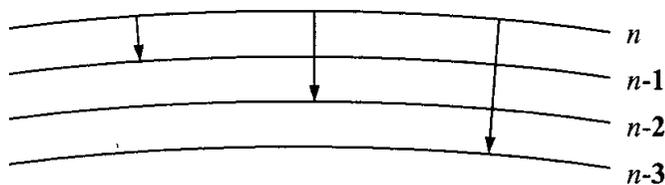
$$a_\tau(n) \cos \omega_\tau(n)t$$



Quantum



$$x(t) = a_1 \cos 1\omega t + a_2 \cos 2\omega t + a_3 \cos 3\omega t$$



Thus, for *large quantum numbers*, the atomic spectrum coincides with a harmonic spectrum

Umdeutung seeks to sharpen the CP, i.e., to find a translation from classical to quantum that is valid for all quantum numbers (not only large n).



Heisenberg's *Umdeutung* (1925)

Assumption: The theory should contain only quantities that are *observable*, which are

transition frequencies ω_{nm} All usual (mechanical) quantities (e.g., x, p)
 amplitudes A_{nm} are *arrays* of these observable quantities $x(t) \rightarrow \sum_{?} A_{nm} e^{i\omega_{nm}t}$

How are frequencies added? $\omega_{nk} + \omega_{km} = K \left[\frac{1}{m^2} - \frac{1}{k^2} + \frac{1}{k^2} - \frac{1}{n^2} \right] = \omega_{nm}$ (Ritz principle)

If terms are represented by $A_{nm} e^{i\omega_{nm}t}$ and frequencies add, amplitudes should multiply. But *how?*

$$A_{nm} e^{i\omega_{nm}t} = \sum_k A_{nk} e^{i\omega_{nk}t} A_{km} e^{i\omega_{km}t}$$

$$A_{nm} = \sum_k A_{nk} A_{km}$$

Matrix multiplication!



Heisenberg's *Umdeutung* (1925)

Classical



Quantum-theoretical

Fourier series

$$x(n, t) = \sum_{-\infty}^{+\infty} \mathfrak{A}_{\alpha}(n) e^{i\omega(n)\alpha t}$$

Eine solche Vereinigung der entsprechenden quantentheoretischen Größen scheint wegen der Gleichberechtigung der Größen $n, n - \alpha$ nicht ohne Willkür möglich und deshalb nicht sinnvoll; wohl aber kann man die Gesamtheit der Größen

$$\mathfrak{A}(n, n - \alpha) e^{i\omega(n, n - \alpha)t}$$

als Repräsentant der Größe $x(t)$ auffassen und dann die oben gestellte Frage zu beantworten suchen: Wodurch wird die Größe $x(t)^2$ repräsentiert?

$x(t)^2$

$$x(t)^2 = \sum_{-\infty}^{+\infty} \mathfrak{B}_{\beta}(n) e^{i\omega(n)\beta t}$$

Quantentheoretisch scheint es die einfachste und natürlichste Annahme, die Beziehungen (3, 4) durch die folgenden zu ersetzen:

$$\mathfrak{B}(n, n - \beta) e^{i\omega(n, n - \beta)t} = \sum_{-\infty}^{+\infty} \mathfrak{A}(n, n - \alpha) \mathfrak{A}(n - \alpha, n - \beta) e^{i\omega(n, n - \beta)t} \quad (7)$$

$x(t)y(t)$

$$\mathfrak{C}_{\beta}(n) = \sum_{-\infty}^{+\infty} \mathfrak{A}_{\alpha}(n) \mathfrak{B}_{\beta - \alpha}(n)$$

$$\mathfrak{C}(n, n - \beta) = \sum_{-\infty}^{+\infty} \mathfrak{A}(n, n - \alpha) \mathfrak{B}(n - \alpha, n - \beta)$$

Während klassisch $x(t) \cdot y(t)$ stets gleich $y(t) x(t)$ wird, braucht dies in der Quantentheorie im allgemeinen nicht der Fall zu sein.



Matrix Mechanics (Born & Jordan)

- *Heisenberg's mathematics is matrix analysis*

The mathematical basis of Heisenberg's treatment is the *law of multiplication* of quantum-theoretical quantities, which he derived from an ingenious consideration of correspondence arguments. The development of his formalism, which we give here, is based upon the fact that this rule of multiplication is none other than the well-known mathematical rule of *matrix multiplication*. The infinite square array (with discrete or continuous indices) which appears at the start of the next section, termed a *matrix*, is a representation of a physical quantity which is given in classical theory as a function of time. The mathematical method of treatment inherent in the new quantum mechanics is thereby characterized through the employment of *matrix analysis* in place of the usual number analysis.



Matrix Mechanics (Born & Jordan)

Recipes (Tomonaga)

Recipe (I): Consider that each quantity is a matrix and that, when the quantity is real-number-like, the matrix is hermitian.

Recipe (II): Assume that the (n, n') element of the matrix of a physical quantity oscillates, as a function of time, as $\exp(2\pi i\nu_{nn'}t)$.

Recipe (III): For the frequencies there is the combination law

$$\nu_{nn'} + \nu_{n'n''} = \nu_{nn''} \quad \nu_{nn} = 0, \quad \text{and} \quad \nu_{nn'} = -\nu_{n'n}$$

Recipe (IV): The time derivative of a physical quantity should be defined by the matrix whose elements are the time derivatives of the corresponding elements of the matrix representing the original quantity.

$$x = \begin{bmatrix} x_{11} & x_{12} & x_{13} \dots \\ x_{21} & x_{22} & x_{23} \dots \\ x_{31} & x_{32} & x_{33} \dots \\ \vdots & \vdots & \vdots \end{bmatrix} \quad v = \begin{bmatrix} \dot{x}_{11} & \dot{x}_{12} & \dot{x}_{13} \dots \\ \dot{x}_{21} & \dot{x}_{22} & \dot{x}_{23} \dots \\ \dot{x}_{31} & \dot{x}_{32} & \dot{x}_{33} \dots \\ \vdots & \vdots & \vdots \end{bmatrix} \quad v = 2\pi i \begin{bmatrix} 0 & \nu_{12}x_{12} & \nu_{13}x_{13} \dots \\ \nu_{21}x_{21} & 0 & \nu_{23}x_{23} \dots \\ \nu_{31}x_{31} & \nu_{32}x_{32} & 0 \dots \\ \vdots & \vdots & \vdots \end{bmatrix} \quad \begin{aligned} v_{nn'} &= (\dot{x})_{nn'} = 2\pi i\nu_{nn'}x_{nn'} \\ (\dot{A})_{nn'} &= 2\pi i\nu_{nn'}A_{nn'} \end{aligned}$$



Matrix Mechanics (Born & Jordan)

Recipes (Tomonaga)

Recipe (V): $(A + B)_{nn'} = A_{nn'} + B_{nn'}$

Recipe (VI): $(AB)_{nn'} = \sum_{n''} A_{nn''} B_{n''n'}$

Recipe (VII): Using the definition of time derivative, sum, and product as given above, insert the coordinates and their time derivatives into the equation of motion characteristic of the given dynamical system.

Newton's 2nd law

$$\ddot{x} + f(x) = 0$$

Hamilton's equations

$$\dot{q} = \frac{\partial H}{\partial p} \quad \dot{p} = -\frac{\partial H}{\partial q}$$

Hamiltonian (energy)

$$H = \frac{1}{2m} p^2 + U(q)$$

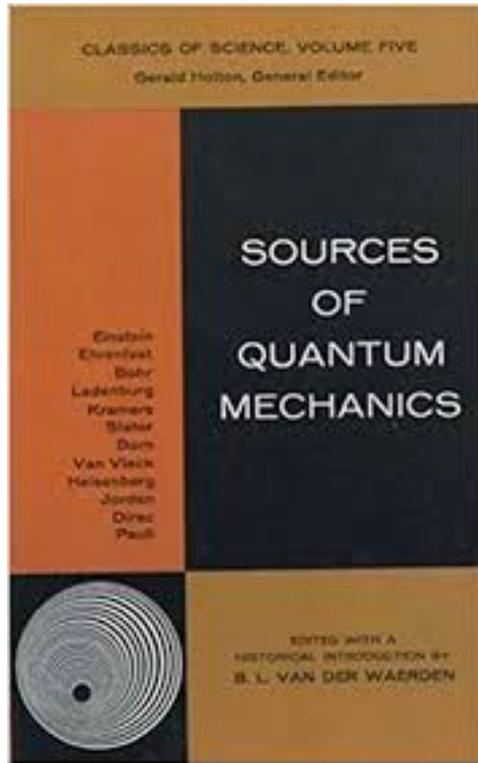
Recipe (VIII): Assume that the momentum p , conjugate to the coordinate q , satisfies the relationship,

$$pq - qp = \frac{h}{2\pi i} \mathbf{1}$$

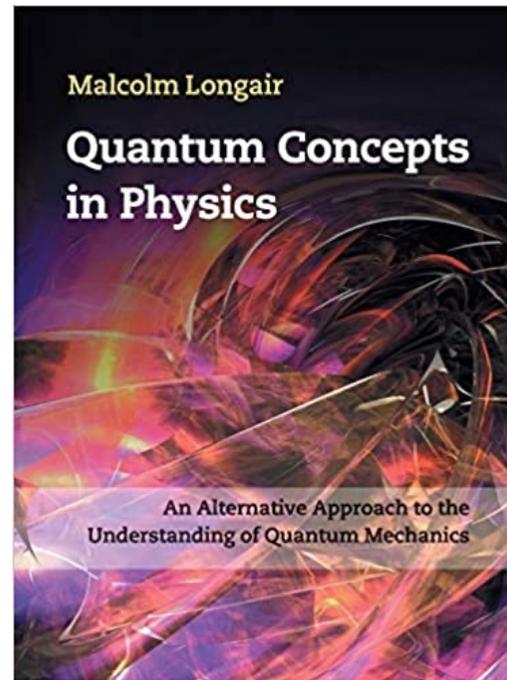
Therefore, we arrive at the conclusion that the matrix H must be a diagonal matrix; i.e.,

$$H_{nn'} = W_n \delta_{nn'}$$

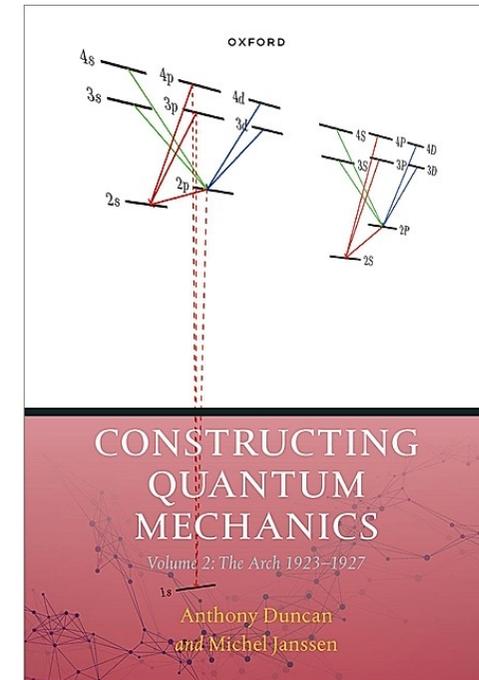
Useful references



Original papers



Didactic reconstruction



Translation as heuristics: Heisenberg's turn to matrix mechanics

Alexander Blum*, Martin Jähnert, Christoph Lehner, Jürgen Renn

Max Planck Institute for the History of Science, Boltzmannstraße 22, 14195 Berlin, Germany

[Studies in History and Philosophy of Modern Physics 60 \(2017\) 3–22](#)

Historical research

Some lessons from case 2)

- Matrices entered quantum mechanics when Heisenberg tried to “sharpen” Bohr’s correspondence principle and found new rules that were consistent with quantum theoretical assumptions like doubly indexed frequencies and the Ritz principle.
- Born & Jordan soon realized that Heisenberg was operating with matrices. In matrix mechanics, physical quantities are represented by matrices (NOT operators), but Hamiltonian mechanics remains valid. The goal was to diagonalize the H matrix to find energy levels.

Three routes to wave mechanics

(1) Gas statistics:

- Schrödinger is unwilling to accept a new statistics for microscopic particles. He reads **de Broglie** and discovers that **Bose-Einstein statistics** can be interpreted as a Boltzmann statistics of standing matter wave modes.

(2) Theoretical spectroscopy:

- De Broglie's explanation of quantum orbits as resonance phenomenon gets picked up enthusiastically by Schrödinger.

(3) Hamilton's optical-mechanical analogy:

- De Broglie's use of the optical-mechanical analogy appeals to Schrödinger because of his own explorations of Hamiltonian mechanics around 1920 and leads him to wave mechanics.

Extending Hamilton's optical-mechanical analogy

Mechanics

Least action (Euler, 1744)

$$\delta \int_A^B 2T dt = 0$$

$$\delta \int_A^B \sqrt{2m(E - V)} ds = 0$$



$$u = \frac{C}{\sqrt{2m(E - V)}}$$

Optics

Least time (Fermat, 1662)

$$\delta \int_A^B \frac{ds}{u} = 0$$

We have made a mental picture of an optical medium, in which the manifold of possible light-rays coincides with the manifold of dynamical orbits of a mass-point m moving with given energy E

$$E = h\nu$$

This enables us to push the analogy a step farther by picturing the dependence on E as **dispersion**, i.e., as a dependence on frequency.

Group velocity

Can we make a small "point-like" light-signal move exactly like our mass-point?

At first sight this seems impossible

$$w = \frac{1}{m} \sqrt{2m(E - V)}$$

$$u = \frac{c}{\sqrt{2m(E - V)}}$$

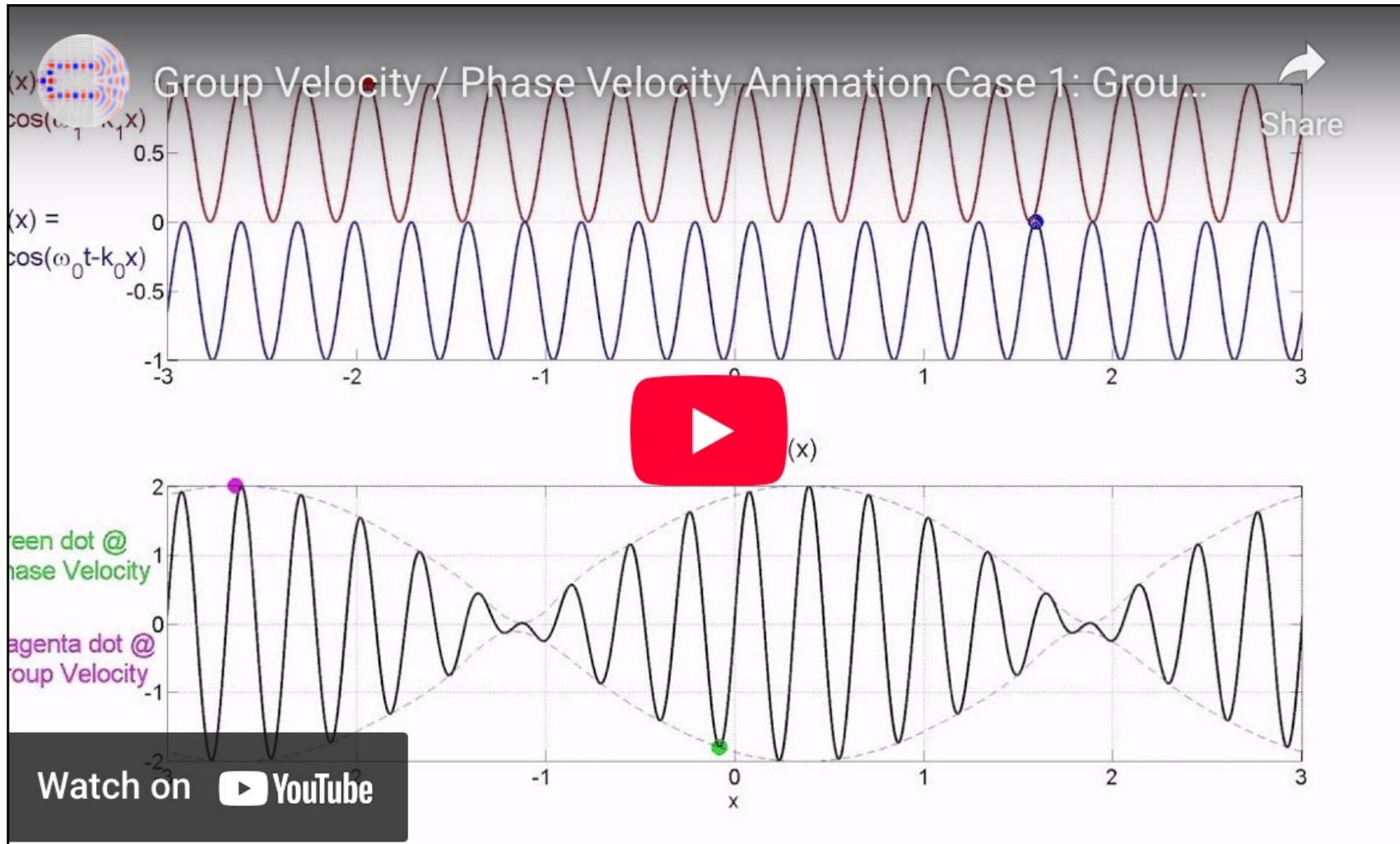
But u is *phase-velocity*. A small light-signal must move with the *group-velocity* g

Group velocity

Trigonometric identity

$$\cos \alpha + \cos \beta = 2 \cos \frac{1}{2}(\alpha + \beta) \cos \frac{1}{2}(\alpha - \beta).$$

Adding two cosines (travelling waves)



Group velocity

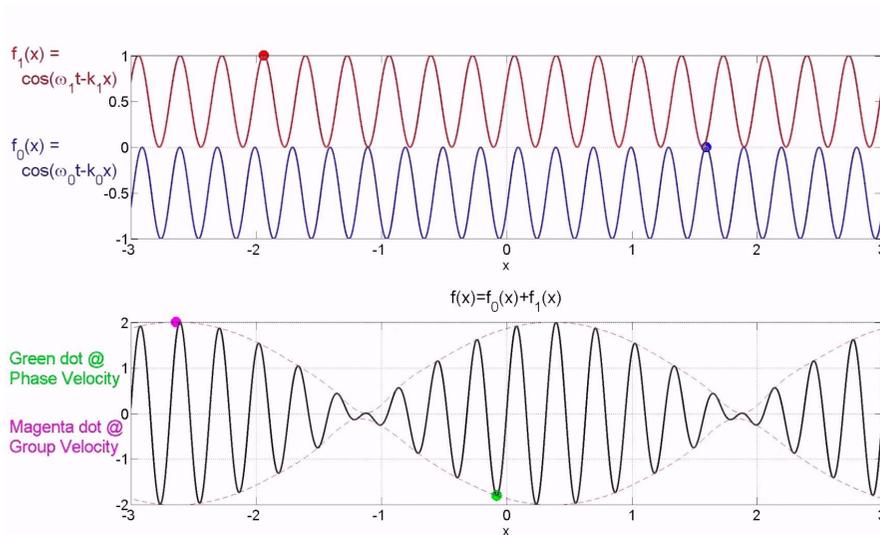
Can we make a small "point-like" light-signal move exactly like our mass-point?

At first sight this seems impossible

$$w = \frac{1}{m} \sqrt{2m(E - V)}$$

$$u = \frac{C}{\sqrt{2m(E - V)}}$$

But u is *phase-velocity*. A small light-signal must move with the *group-velocity* g



$$\frac{1}{g} = \frac{d}{dv} \left(\frac{v}{u} \right)$$

$$\frac{1}{g} = \frac{d}{dE} \left(\frac{E}{u} \right)$$

We will try to make $g = w$

$$u = \frac{E}{\sqrt{2m(E - V)}}$$

Wave equation

$$\nabla^2 p - \frac{1}{u^2} \ddot{p} = 0$$

Wave equation

$$p(x, y, z, t) = \psi(x, y, z) e^{2\pi i \nu t}$$

Profile oscillates with frequency ν

$$\nabla^2 \psi + \frac{4\pi^2 \nu^2}{u^2} \psi = 0$$

Amplitude equation

$$u = \frac{E}{\sqrt{2m(E - V)}}$$

So that $g = w!$

$$\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

Time-independent SE

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\mathbf{x}) \psi = E \psi$$

Born's ("trivial") derivation of Schrödinger's equation

Amplitude equation

$$\frac{\partial^2}{\partial x^2} \psi(x) + \frac{4\pi^2}{\lambda^2} \psi(x) = 0$$

$$\frac{\partial^2}{\partial x^2} \psi(x) + \frac{4\pi^2 p^2}{h^2} \psi(x) = 0$$

$$\frac{\partial^2}{\partial x^2} \psi(x) + \frac{8m\pi^2(E - V)}{h^2} \psi(x) = 0$$

$$\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

De Broglie

$$p = h/\lambda$$

Classically

$$p = \sqrt{2m(E - V)}$$

Time-dependent wave equation

$$\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0, \quad (13)$$

$$\psi \sim e^{\frac{2\pi i E t}{h}} \dots (21)$$

[we need] to remove the parameter E from the amplitude equation and introduce time derivatives instead. This is easily done. Take one of the family (13) (with a particular value of E), then by (21) we have

$$\dot{\psi} = \frac{2\pi i E}{h} \psi \quad \text{or} \quad E \psi = \frac{h}{2\pi i} \dot{\psi}$$

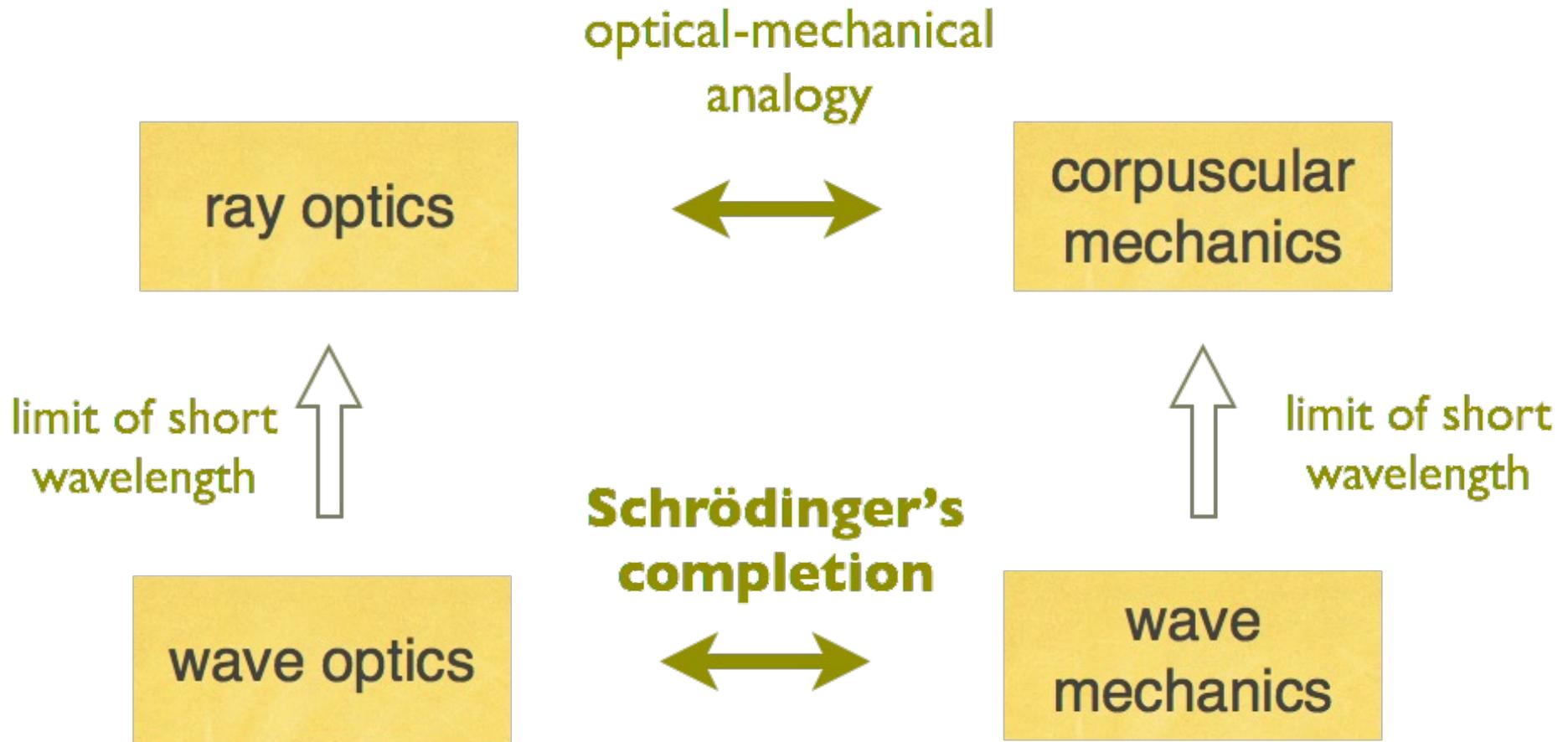
Using this, we get from (13)

$$\nabla^2 \psi - \frac{4\pi m i}{h} \dot{\psi} - \frac{8\pi^2 m V}{h^2} \psi = 0. \quad (22)$$

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[\frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t)$$

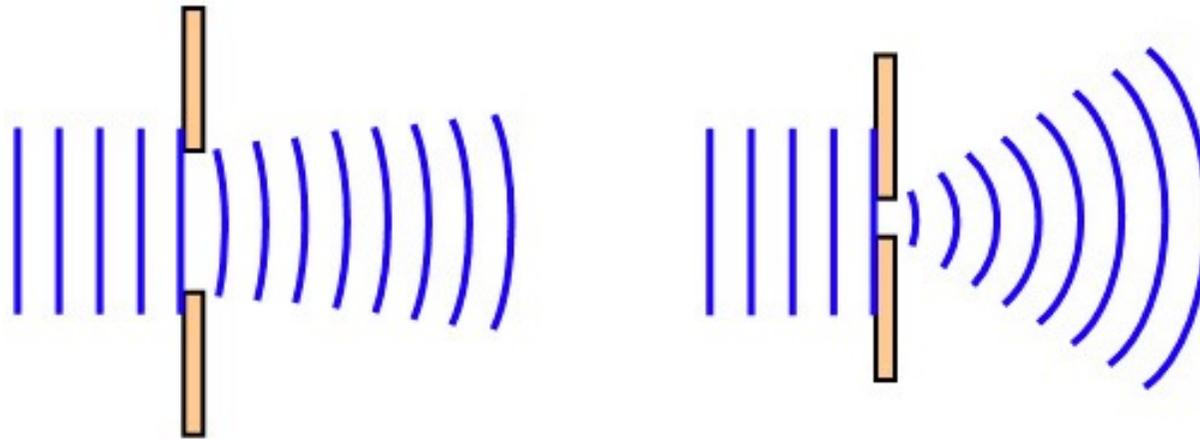


Schrödinger's analogy/completion



Corpuscular mechanics is merely a limiting case of a more general wave mechanics!

Schrödinger's analogy/completion

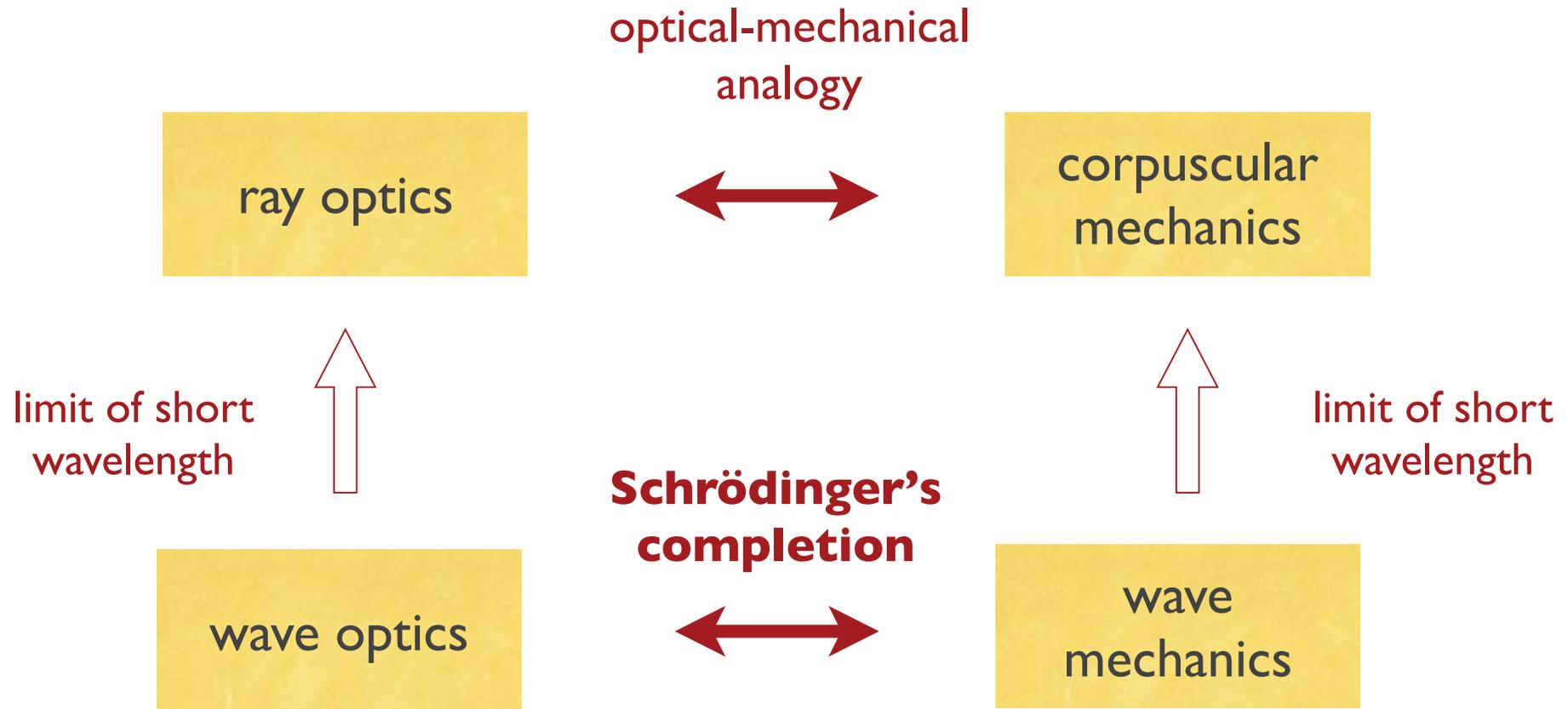


The step which leads from ordinary mechanics to wave mechanics is an advance similar in kind to Huygens' theory of light, which replaced Newton's theory.

Ordinary mechanics : Wave mechanics = Geometrical optics : Undulatory optics.

Typical quantum phenomena are analogous to typical wave phenomena like diffraction and interference.

Schrödinger's Completion of Hamilton's Analogy

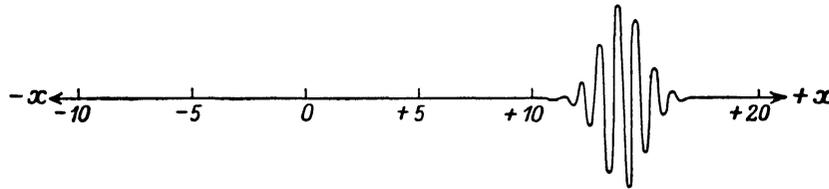


Corpuscular mechanics is merely a limiting case of a more general wave mechanics!

Some lessons from case 3.1)

- Schrödinger's original derivation combined 3 elements:
 1. Hamilton's optical-mechanical analogy
 2. $E = h\nu$
 3. Particle velocity = Group velocity
- Time-dependent was derived later, substituting the parameter E by the time derivative of ψ .
- Schrödinger's overarching goal was to complete Hamilton's optical-mechanical analogy. Corpuscular mechanics is a limiting case of a *more general wave mechanics*!

Complex numbers in the birth of wave mechanics



$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$$

Why is the wave function complex?

Griffiths p.1

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi.$$

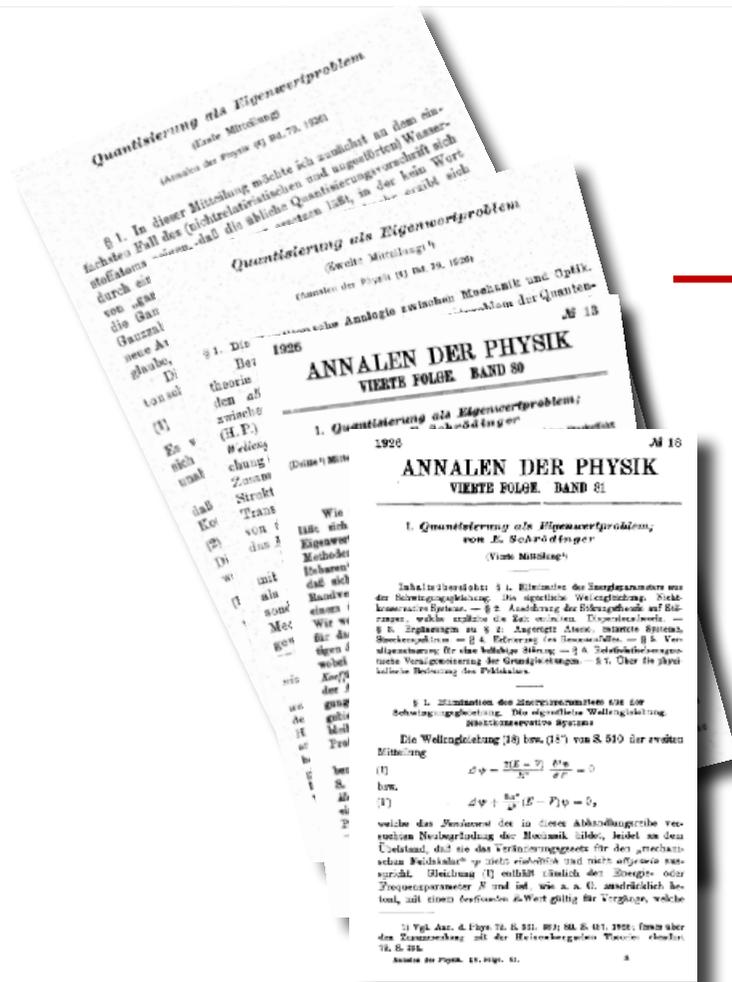
p.2

$$|\Psi(x, t)|^2 dx = \left\{ \begin{array}{l} \text{probability of finding the particle} \\ \text{between } x \text{ and } (x + dx), \text{ at time } t. \end{array} \right\}$$

Schrödinger

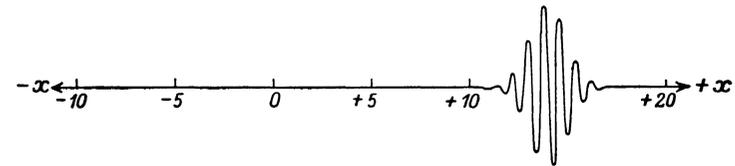
What is unpleasant here, and indeed directly to be objected to, is the use of complex numbers. ψ is fundamentally a real function (Schrödinger to Lorentz on June 6, 1926)

Schrödinger's struggles with a complex ψ



The Continuous Transition from Micro- to Macro-Mechanics

(Die Naturwissenschaften, 28, pp. 664-666, 1926)

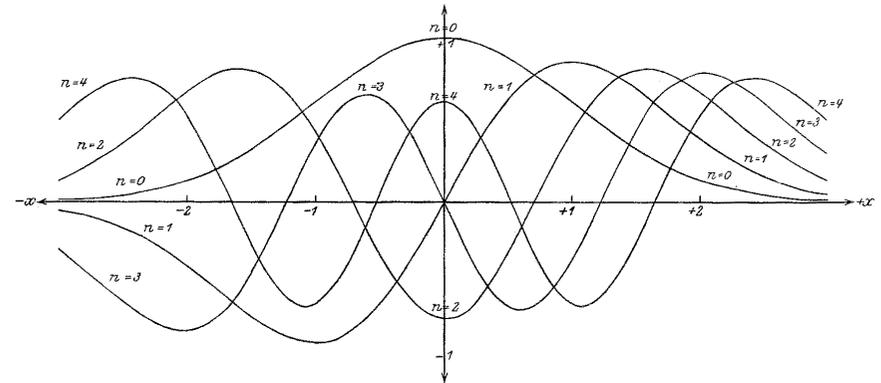


Schrödinger's four communications (1926)

Taking the real part of ψ

The Continuous Transition from Micro-
to Macro-Mechanics

(*Die Naturwissenschaften*, 28, pp. 664-666, 1926)



Harmonic oscillator

$$\begin{cases} \psi_n = e^{-\frac{x^2}{2}} H_n(x) e^{2\pi i \nu_n t} \\ (\nu_n = \frac{2n+1}{2} \nu_0 ; n = 0, 1, 2, 3 \dots) \end{cases}$$

“A group of proper vibrations
may represent a particle”

$$\psi = \sum_{n=0}^{\infty} \left(\frac{A}{2}\right)^n \frac{\psi_n}{n!} \quad \psi = e^{\pi i \nu_0 t - \frac{A^2}{4}} e^{\frac{1}{2} \pi i \nu_0 t} + A x e^{2\pi i \nu_0 t - \frac{x^2}{2}}$$

Now we take, as is provided for,
the real part of the right-hand side

⁵ i means $\sqrt{-1}$. On the right-hand side
the real part is to be taken, as usual.

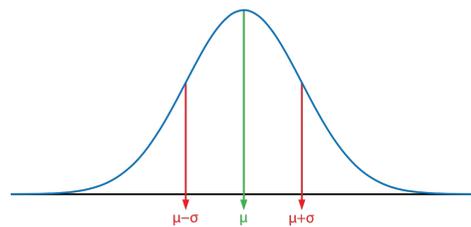
$$\psi = e^{\frac{A^2}{4} - \frac{1}{2}(x - A \cos 2\pi \nu_0 t)^2} \cos \left[\pi \nu_0 t + (A \sin 2\pi \nu_0 t) \cdot \left(x - \frac{A}{2} \cos 2\pi \nu_0 t\right) \right]$$

$$\psi = e^{\frac{A^2}{4} - \frac{1}{2}(x - A \cos 2\pi\nu_0 t)^2} \cos \left[\pi\nu_0 t + (A \sin 2\pi\nu_0 t) \cdot \left(x - \frac{A}{2} \cos 2\pi\nu_0 t \right) \right]$$

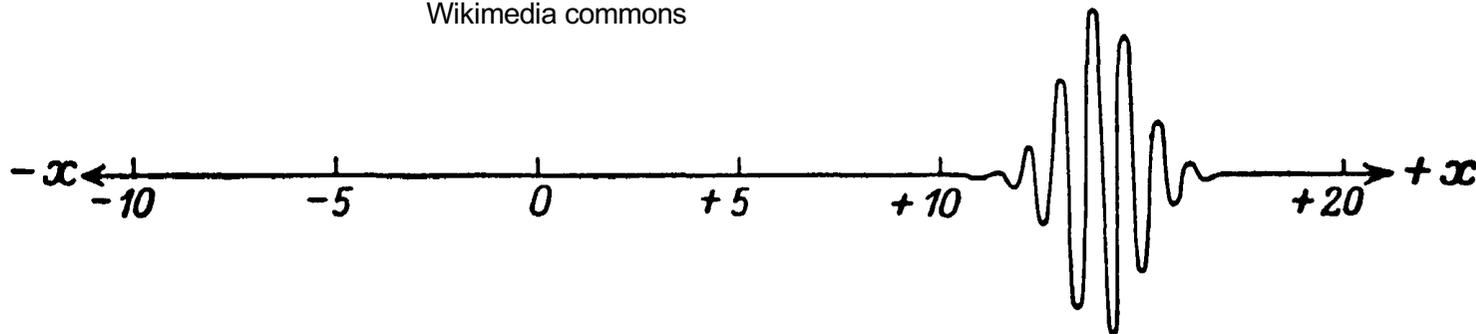
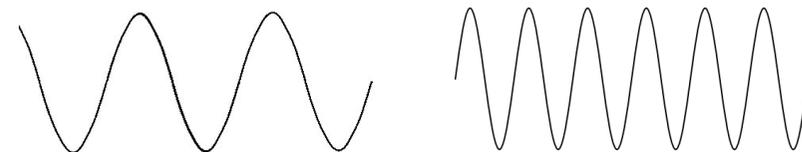
$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

Gaussian

cosine wave with varying period

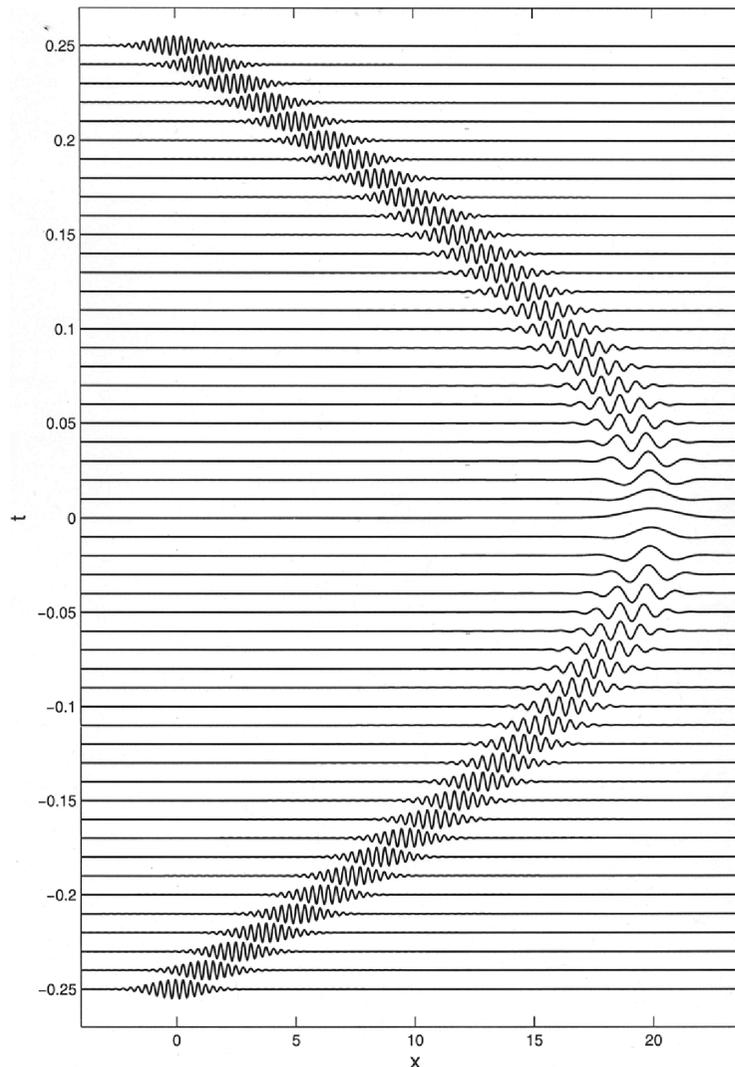


Wikimedia commons



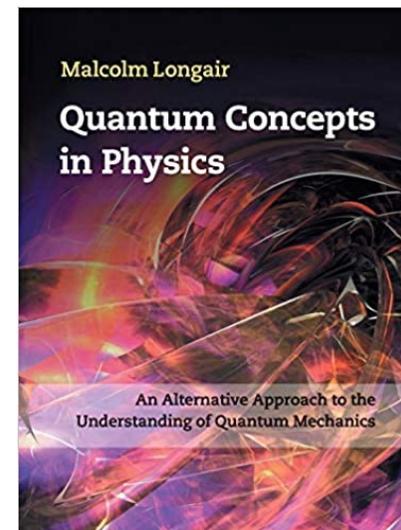
Oscillating wave group as the representation of a particle in wave mechanics

$$\psi = e^{\frac{A^2}{4} - \frac{1}{2}(x - A \cos 2\pi\nu_0 t)^2} \cos \left[\pi\nu_0 t + (A \sin 2\pi\nu_0 t) \cdot \left(x - \frac{A}{2} \cos 2\pi\nu_0 t \right) \right]$$

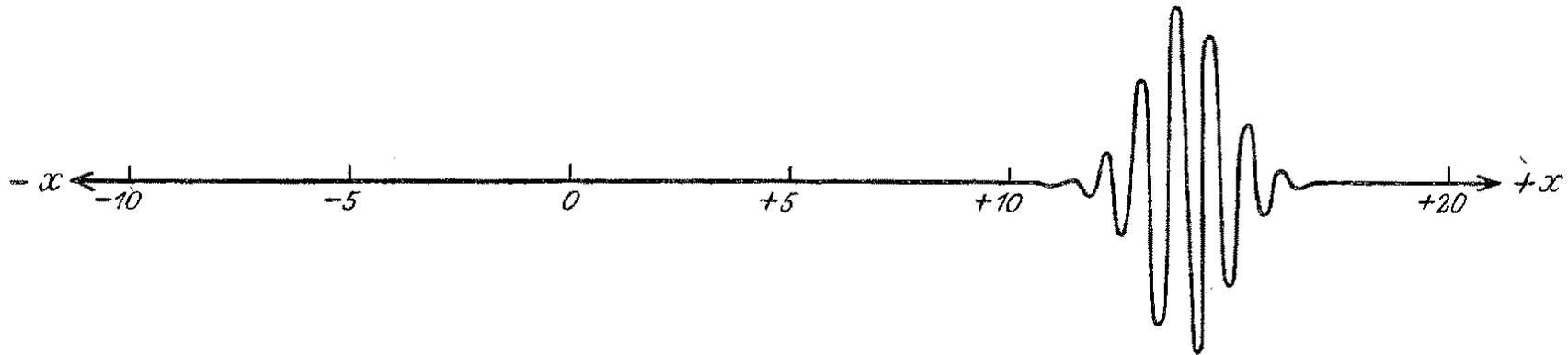


The evolution of wave-packet with A = 20
(Diagram created by Dr. David Green)

Source: Chapter 14.6

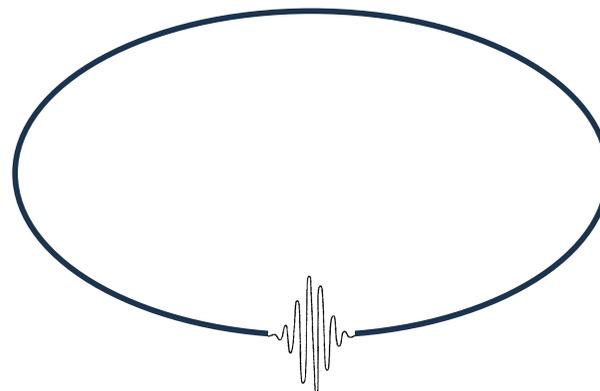


Zoom in: Particles are wave groups



A bold prediction

We can definitely foresee that, in a similar way, wave groups can be constructed which move round highly quantised Kepler ellipses and are the representation by wave mechanics of the hydrogen electron.



Avoiding i in the TDSE

4th communication: Eliminate the E parameter from the TI equation $\nabla^2\psi + \frac{8\pi^2}{h^2}(E - V)\psi = 0$

$$\psi \sim \text{real part of } \left(e^{\pm \frac{2\pi i E t}{h}} \right), \text{ which leads to } \frac{\partial^2 \psi}{\partial t^2} = -\frac{4\pi^2 E^2}{h^2} \psi$$

Square the TI equation and substitute $\left(\nabla^2 - \frac{8\pi^2}{h^2} V \right)^2 \psi + \frac{16\pi^2}{h^2} \frac{\partial^2 \psi}{\partial t^2} = 0$

*This is the uniform and general **wave equation for the scalar field ψ** . It is no longer of the simple type, but is of the **fourth order**, similar to some in elasticity (vibrating plate)*

Accepting and justifying a complex ψ

- *The Exchange of Energy according to Wave Mechanics* (1927)

$$\nabla^2\psi - \frac{8\pi^2}{h^2}V\psi - \frac{4\pi i}{h}\dot{\psi} = 0$$

Footnote: The wave function must be essentially complex

- 4 Lectures (1928): The problem is to remove the parameter E from the amplitude equation and introduce time derivatives instead. **This is easily done.**

$$\nabla^2\psi + \frac{8\pi^2}{h^2}(E - V)\psi = 0 \quad \psi \sim e^{\frac{2\pi i E t}{h}} \quad \dot{\psi} = \frac{2\pi i E}{h}\psi$$

- No problem with a complex wave function is mentioned
- No discussion about “real” and “imaginary” parts of ψ

Accepting and justifying a complex ψ

Is it possible to ascribe a definite physical meaning to the quantity ψ in such a way that the emission of light with frequencies $\nu_{kk'} = \nu_k - \nu_{k'}$ becomes intelligible? Yes, it is, but - strange to say - **only if we make use of the *complex* ψ -function** as it stands, **instead of its real part**, as we are accustomed to do in ordinary vibration problems.

$$\psi\bar{\psi} = \sum_{k=0}^{\infty} \sum_{k'=0}^{\infty} c_k c_{k'} u_k u_{k'} e^{2\pi i(\nu_k - \nu_{k'})t} \quad \rho = -e\psi\bar{\psi}$$

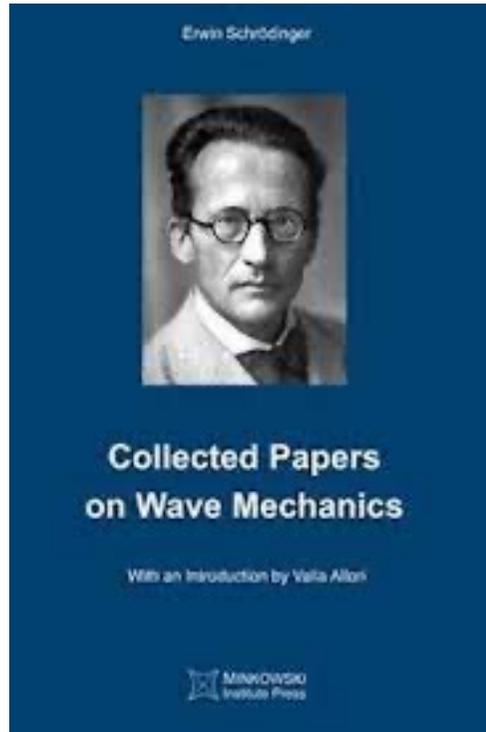
Accepting and justifying a complex ψ

But if the physical meaning is on $\psi\bar{\psi}$, why not replace the wave equation by an equation which describes the behaviour of $\psi\bar{\psi}$ directly?

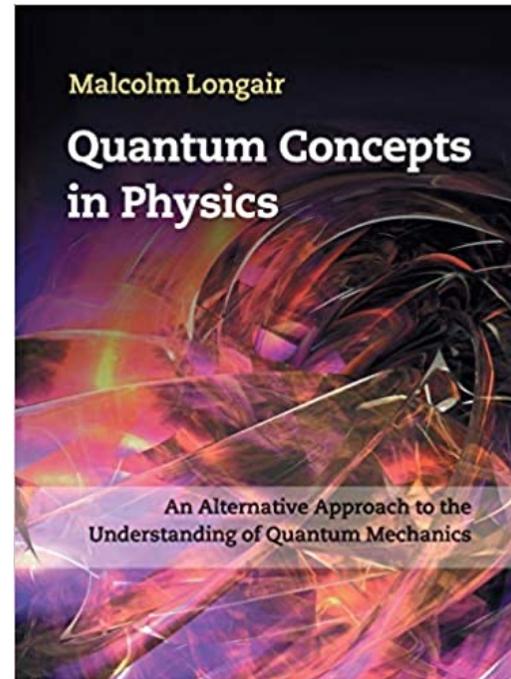
Maxwell's equations describe the behaviour of **electromagnetic vectors**. **But these are not really accessible to observation**. [...] all observable quantities (energy, Maxwellian-stresses) are **quadratic functions of the field-vectors**.

We might desire to replace Maxwell's equations by others, that determine the observable quadratic functions of the field-vectors directly. But this would mean an **immense complication** and that it would not really be possible to do without Maxwell's equations.

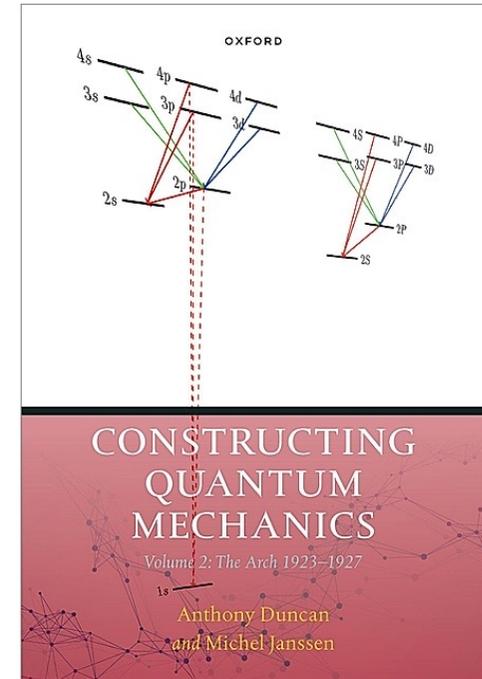
Useful references



Original papers



Didactic reconstruction



The classical roots of wave mechanics: Schrödinger's transformations of the optical-mechanical analogy

Christian Joas, Christoph Lehner*

Max Planck Institute for the History of Science, Boltzmannstr. 22, 14195 Berlin, Germany

Studies in History and Philosophy of Modern Physics 40 (2009) 338-351

Historical research

Some lessons from case 3.2)

- Schrödinger was initially looking for physical meaning of the *real* component of his wave function.
- An awareness of Schrödinger's original struggles to accept a complex wave function could be comforting for students who are puzzled by a complex *psi*.
- Why not discuss Schrödinger's micro-macro paper when solving the quantum harmonic oscillator in QM courses?

Zur Quantenmechanik der Stoßvorgänge.

[Vorläufige Mitteilung.¹⁾]

Von **Max Born**, Göttingen.

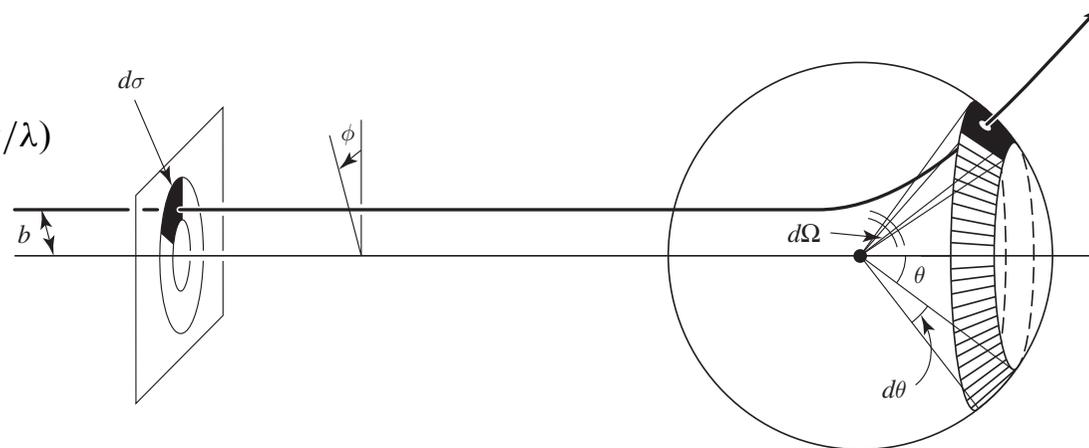
(Eingegangen am 25. Juni 1926.)

Assumption: Definite states *before* and *after* collision

After?

Before

$$\psi_{nE}^0(q, z) = \psi_n^0(q) \sin(2\pi z/\lambda)$$



$$\psi_{nr}^1(x, y, z; q_k) = \sum_m \iint_{\alpha x + \beta y + \gamma z > 0} d\omega \Phi_{n,m}(\alpha, \beta, \gamma) \sin k_{n,m}(\alpha x + \beta y + \gamma z + \delta) \psi_m^0(q_k)$$

Zur Quantenmechanik der Stoßvorgänge.

[Vorläufige Mitteilung.¹⁾]

Von **Max Born**, Göttingen.

(Eingegangen am 25. Juni 1926.)

Overview

- Heisenberg's QM is applied only to (periodic) stationary states, what about (aperiodic) transitions?
- Collision processes (scattering) are crucial and should be described by the QM formalism.
- "Of the different forms of the theory only Schrödinger's has proved suitable for this process, and for this reason I might regard it as the deepest formulation of the quantum laws."
- Assumption: Definite states before and after collision

ON THE QUANTUM MECHANICS OF COLLISIONS

[Preliminary communication][†]

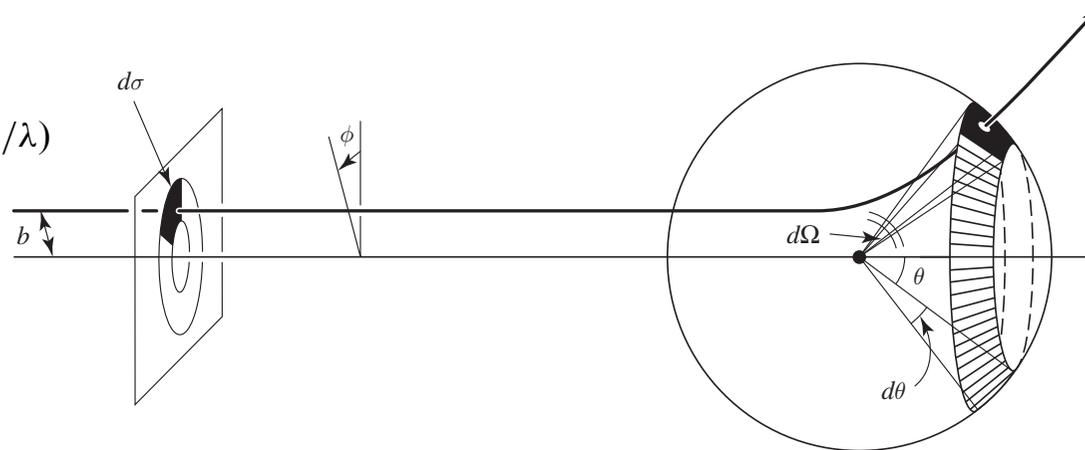
MAX BORN

Assumption: Definite states *before* and *after* collision

After?

Before

$$\psi_{nE}^0(q, z) = \psi_n^0(q) \sin(2\pi z/\lambda)$$



The task is clear:

- Solve the Schrödinger wave equation for the system atom-plus-electron
- Boundary condition: solution in a preselected direction of electron space goes over asymptotically to a plane wave exactly in this direction (arriving electron)
- The unperturbed electron corresponds to eigenfunctions $\sin(2\pi/\lambda) (\alpha x + \beta y + \gamma z + \delta)$

ON THE QUANTUM MECHANICS OF COLLISIONS

[Preliminary communication][†]

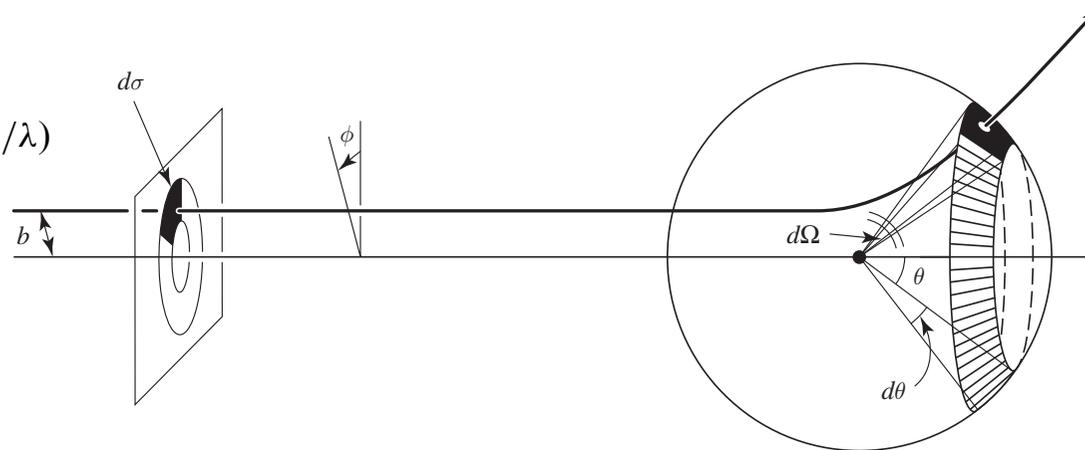
MAX BORN

Assumption: Definite states *before* and *after* collision

After?

Before

$$\psi_{nE}^0(q, z) = \psi_n^0(q) \sin(2\pi z/\lambda)$$



Result: The scattered wave created by this perturbation has asymptotically at infinity the form

$$\psi_{nr}^1(x, y, z; q_k) = \sum_m \iint_{\alpha x + \beta y + \gamma z > 0} d\omega \Phi_{n,m}(\alpha, \beta, \gamma) \sin k_{n,m}(\alpha x + \beta y + \gamma z + \delta) \psi_m^0(q_k)$$

ON THE QUANTUM MECHANICS OF COLLISIONS

[Preliminary communication][†]

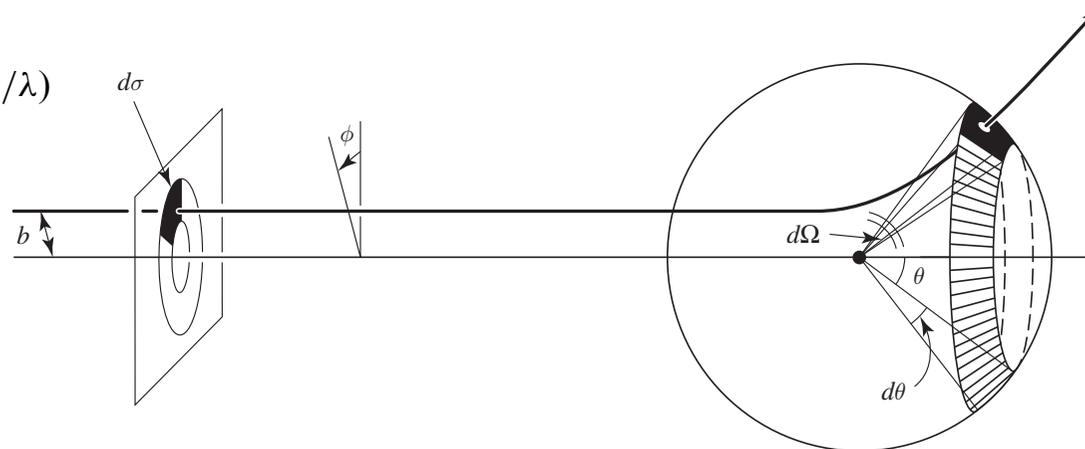
MAX BORN

After

Before

$$\psi_{n\tau}^1(x, y, z; q_k) = \sum_m \iint_{\alpha x + \beta y + \gamma z > 0} d\omega \Phi_{n,\tau m}(\alpha, \beta, \gamma) \sin k_{n,\tau m}(\alpha x + \beta y + \gamma z + \delta) \psi_m^0(q_k)$$

$$\psi_{nE}^0(q, z) = \psi_n^0(q) \sin(2\pi z/\lambda)$$



If one wants to interpret this result in terms of particles rather than waves, then there is *only one* interpretation possible: $\phi_{n\tau m}(\alpha, \beta, \gamma)$ gives the **probability*** that the electron coming in from the z direction will be thrown into the direction determined by α, β and γ (and with a phase of δ).

*Addition in proof: More careful considerations show that probability is proportional to the **square** of $\phi_{n\tau m}(\alpha, \beta, \gamma)$

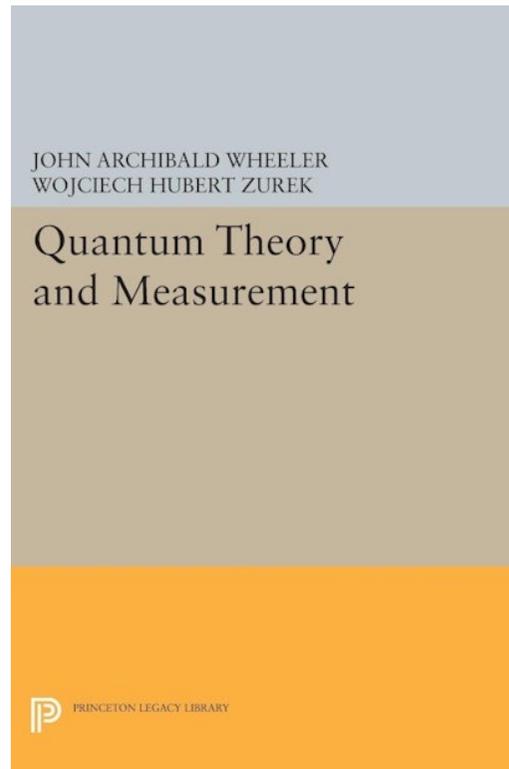
$$\psi_{nr}^1(x, y, z; q_k) = \sum_m \iint_{\alpha x + \beta y + \gamma z > 0} d\omega \Phi_{n,m}(\alpha, \beta, \gamma) \sin k_{n,m}(\alpha x + \beta y + \gamma z + \delta) \psi_m^0(q_k)$$

Die Schrödingersche Quantenmechanik gibt also auf die Frage nach dem Effekt eines Zusammenstoßes eine ganz bestimmte Antwort; aber es handelt sich um keine Kausalbeziehung. Man bekommt keine Antwort auf die Frage, „wie ist der Zustand nach dem Zusammenstoße“, sondern nur auf die Frage, „wie wahrscheinlich ist ein vorgegebener Effekt des Zusammenstoßes“ (wobei natürlich der quantenmechanische Energie-

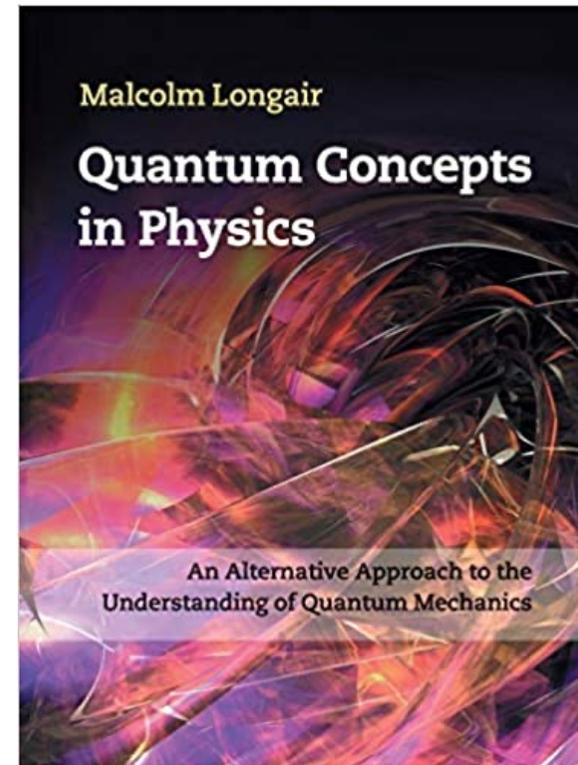
$$\psi_{nr}^1(x, y, z; q_k) = \sum_m \iint_{\alpha x + \beta y + \gamma z > 0} d\omega \Phi_{n,m}(\alpha, \beta, \gamma) \sin k_{n,m}(\alpha x + \beta y + \gamma z + \delta) \psi_m^0(q_k)$$

Hier erhebt sich die ganze Problematik des Determinismus. Vom Standpunkt unserer Quantenmechanik gibt es keine Größe, die im Einzelfalle den Effekt eines Stoßes kausal festlegt; aber auch in der Erfahrung haben wir bisher keinen Anhaltspunkt dafür, daß es innere Eigenschaften der Atome gibt, die einen bestimmten Stoßerfolg bedingen. Sollen wir hoffen, später solche Eigenschaften (etwa Phasen der inneren Atombewegungen) zu entdecken und im Einzelfalle zu bestimmen? Oder sollen wir glauben, daß die Übereinstimmung von Theorie und Erfahrung in der Unfähigkeit, Bedingungen für den kausalen Ablauf anzugeben, eine prästabilisierte Harmonie ist, die auf der Nichtexistenz solcher Bedingungen beruht? Ich selber neige dazu, die Determiniertheit in der atomaren Welt aufzugeben. Aber das ist eine philosophische Frage, für die physikalische Argumente nicht allein maßgebend sind.

Useful references



Original papers



Didactic reconstruction

What Was Born's Statistical Interpretation?

Author(s): Linda Wessels

Source: *PSA: Proceedings of the Biennial Meeting of the Philosophy of Science Association*, Vol. 1980, Volume Two: Symposia and Invited Papers (1980), pp. 187-200

Historical research

Some lessons from case 4)

- Born's statistical interpretation was formulated in the context of the scattering problem where probabilities emerge naturally.
- Einstein's "ghost field": the waves may only be seen as guiding the way for corpuscular light quanta, determining the probability that one light quantum, which is the carrier of energy and momentum, chooses a particular path. The field itself, however, does not have energy or momentum.
- One could summarize approximately, somewhat paradoxically: The movement of particles follows a probability law, the probability itself however evolves in accordance with the law of causality.