

# Erwin Schrödinger and the Genesis of Wave Mechanics

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Niels Bohr Archive

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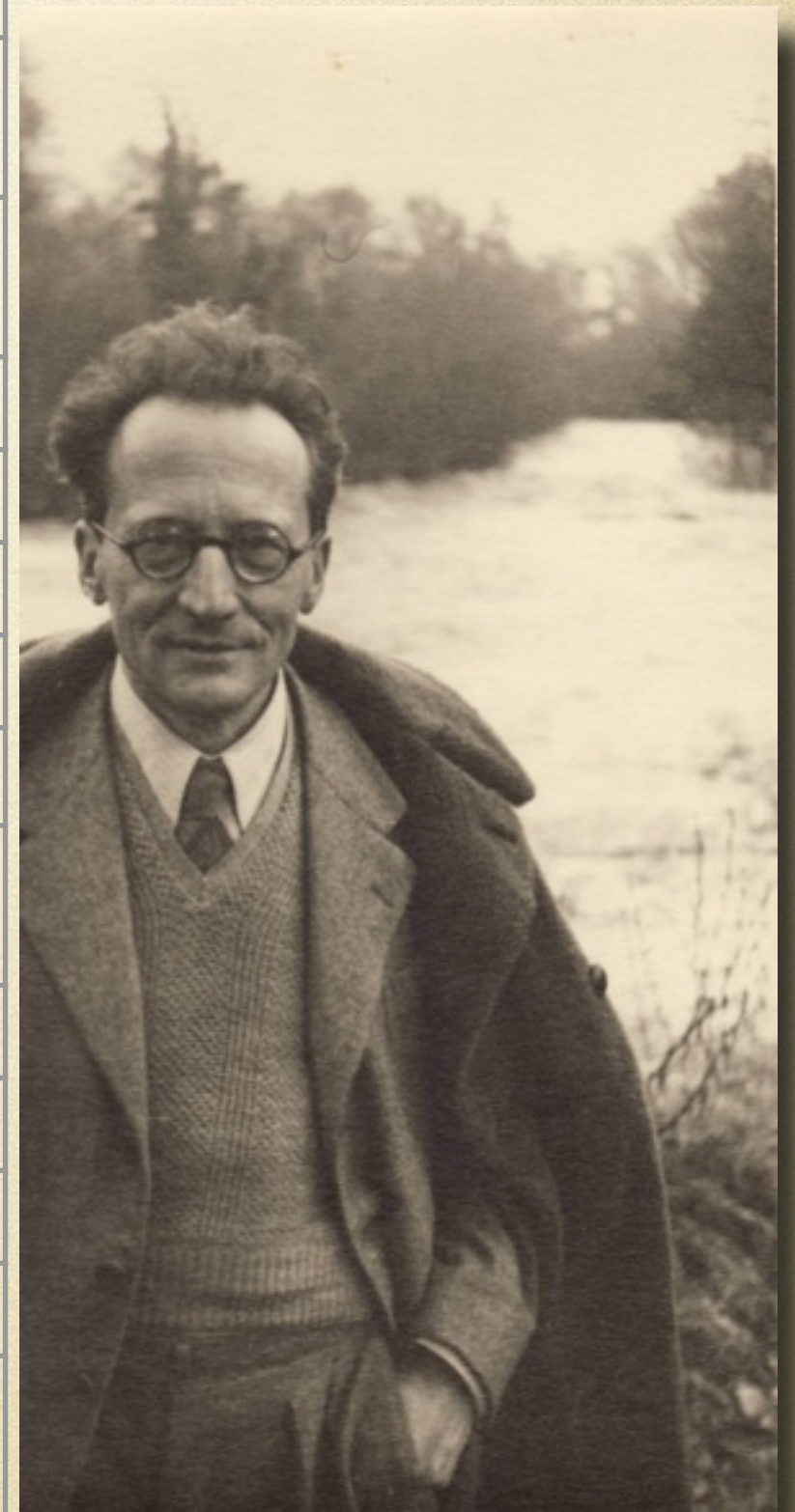





# Erwin Schrödinger (1887-1961)



1887	born in Vienna
1898– 1906	<i>Akademisches Gymnasium</i>
1906– 1910	Vienna University
1910	PhD
1914	Habilitation
1914-1918	military service
1921	Zürich appointment
<b>1926</b>	<b>wave mechanics</b>
1927	Max Planck's successor in Berlin
1933-1936	Oxford
1936-1938	Vienna
1938-1955	Dublin
1955	return to Vienna
1961	death in Vienna, buried in Alpbach/ Tyrol







A photograph of a gravestone for Erwin and Annemarie Schrödinger. The stone is dark with a gold-colored border and a circular medallion at the top. The medallion contains the Schrödinger equation. The main body of the stone contains the names and birth/death dates of the couple, followed by the word 'RIP' in a stylized font. The stone is set against a light-colored wall with some foliage in the background.

$$i\hbar\psi = H\psi$$

Erwin Schrödinger

\* 12.VIII.1887 + 4.I.1961

Annemarie Schrödinger

\* 31.XII.1896 + 3.X.1965

... R i p ...



# Schrödinger's wave equation

“I have been reading your communication like a curious child who eagerly listens to the solution of a riddle it has struggled with for a long time. And I rejoice over the beauties that my eyes discover, which I must, however, study in much greater detail in order to grasp them in their entirety.”

**Max Planck to Schrödinger (1926)**

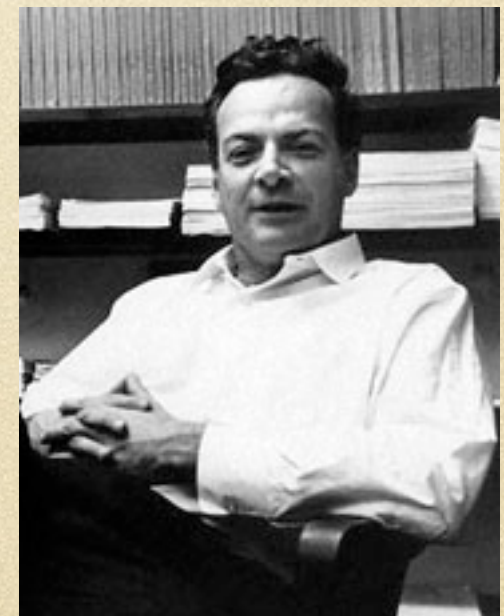


“I just received a submission by Schrödinger to *Annalen [der Physik]*. Schr[ödinger] seems to find the exact same results as Heisenberg and you, but in a completely different, totally crazy way: no matrix algebra, but boundary-value problems.”

**Arnold Sommerfeld to Wolfgang Pauli (1926)**

“Where did we get that from? Nowhere! It is not possible to derive from anything you know. It came out of the mind of Schrödinger, invented in his struggle to find an understanding of the experimental observation of the real world.”

**Richard P. Feynman (1965)**





# Part I:

Quantum theory and the crisis of the  
mechanical worldview



# Quantum theory and the crisis of the mechanical worldview: **19th century physical theories**

- **Mechanics**
- **Electrodynamics**
- **Thermodynamics**

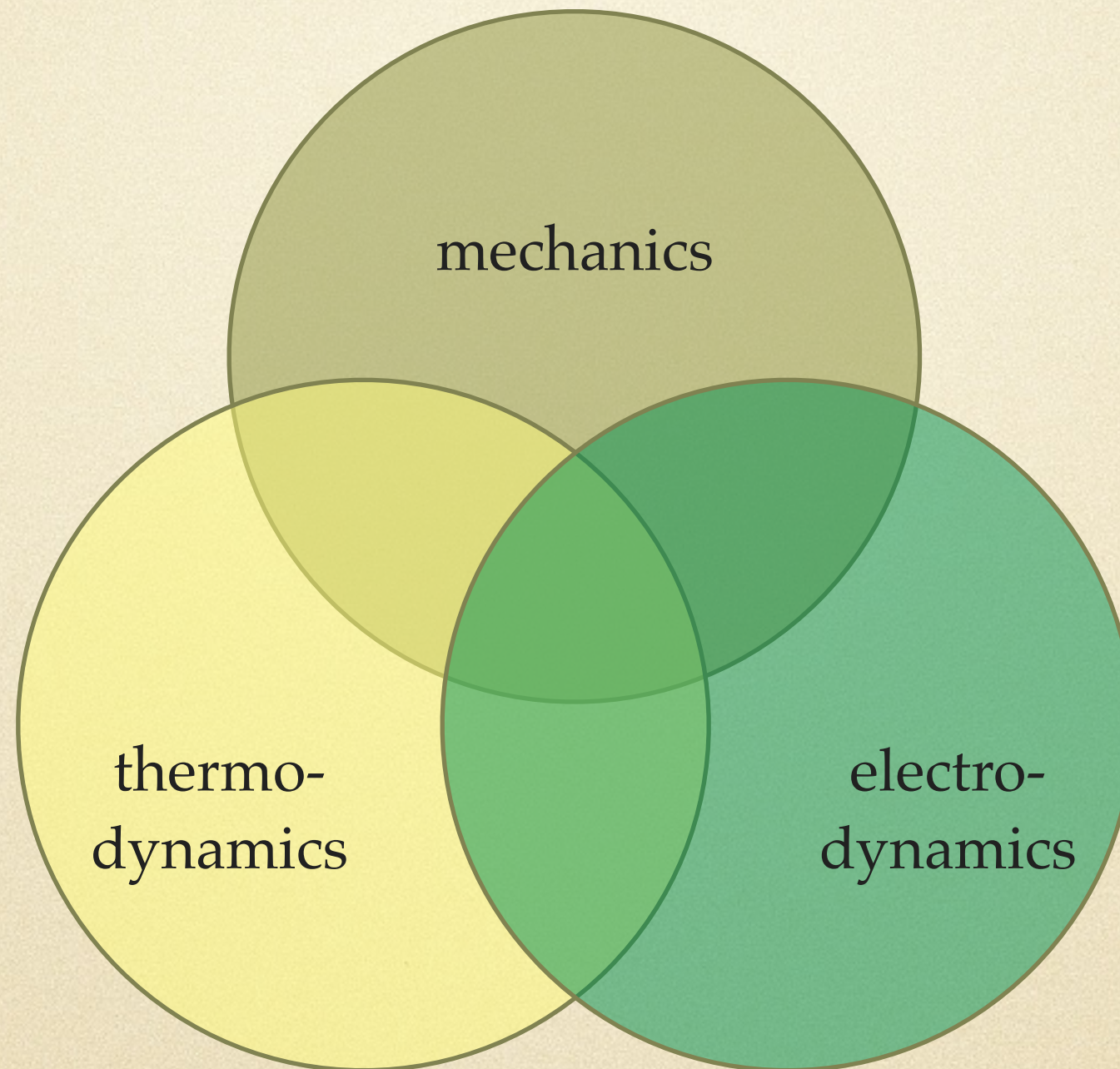


Solvay 1911



Quantum theory and the crisis of the mechanical worldview:

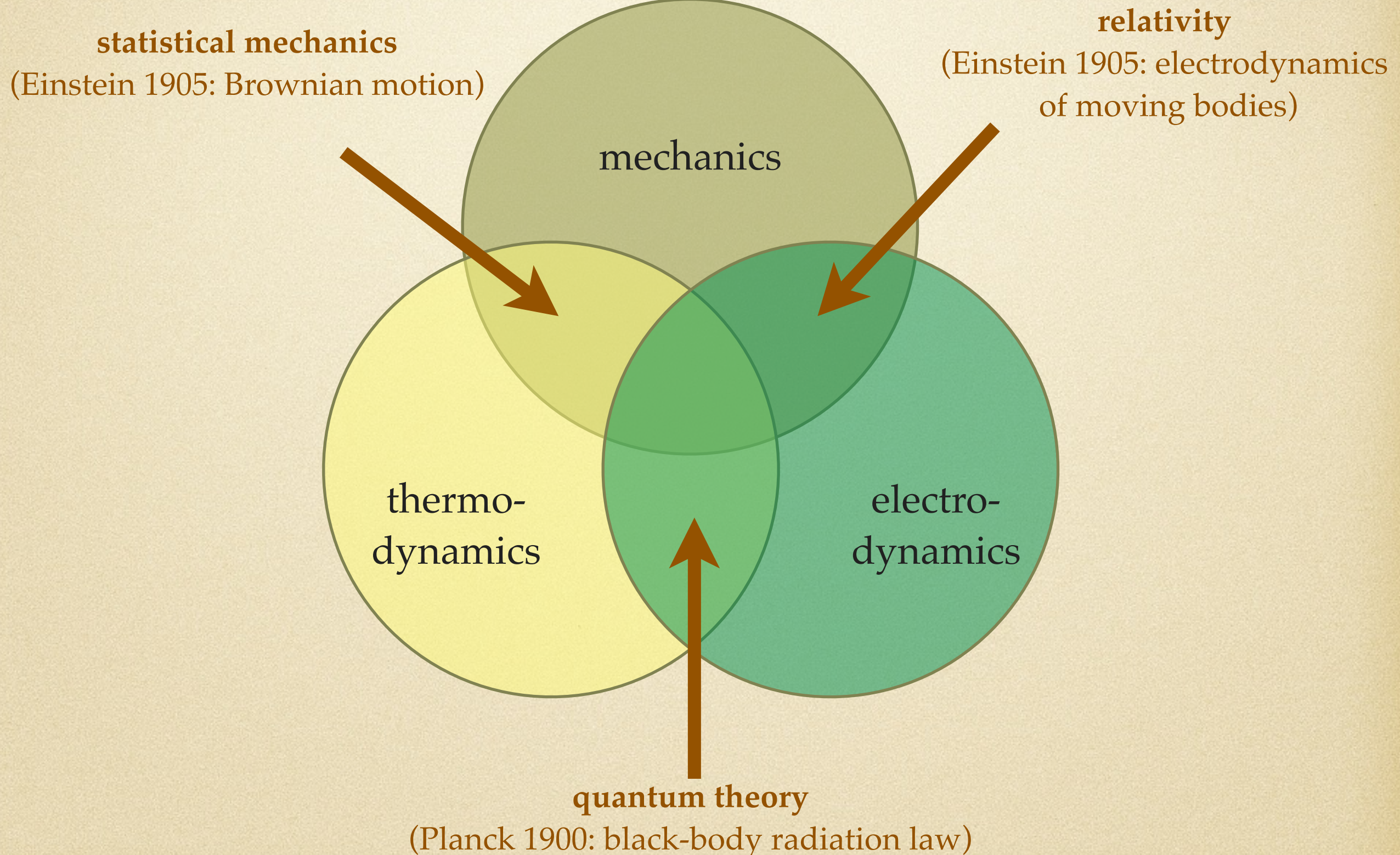
## **Borderline Problems**





# Quantum theory and the crisis of the mechanical worldview:

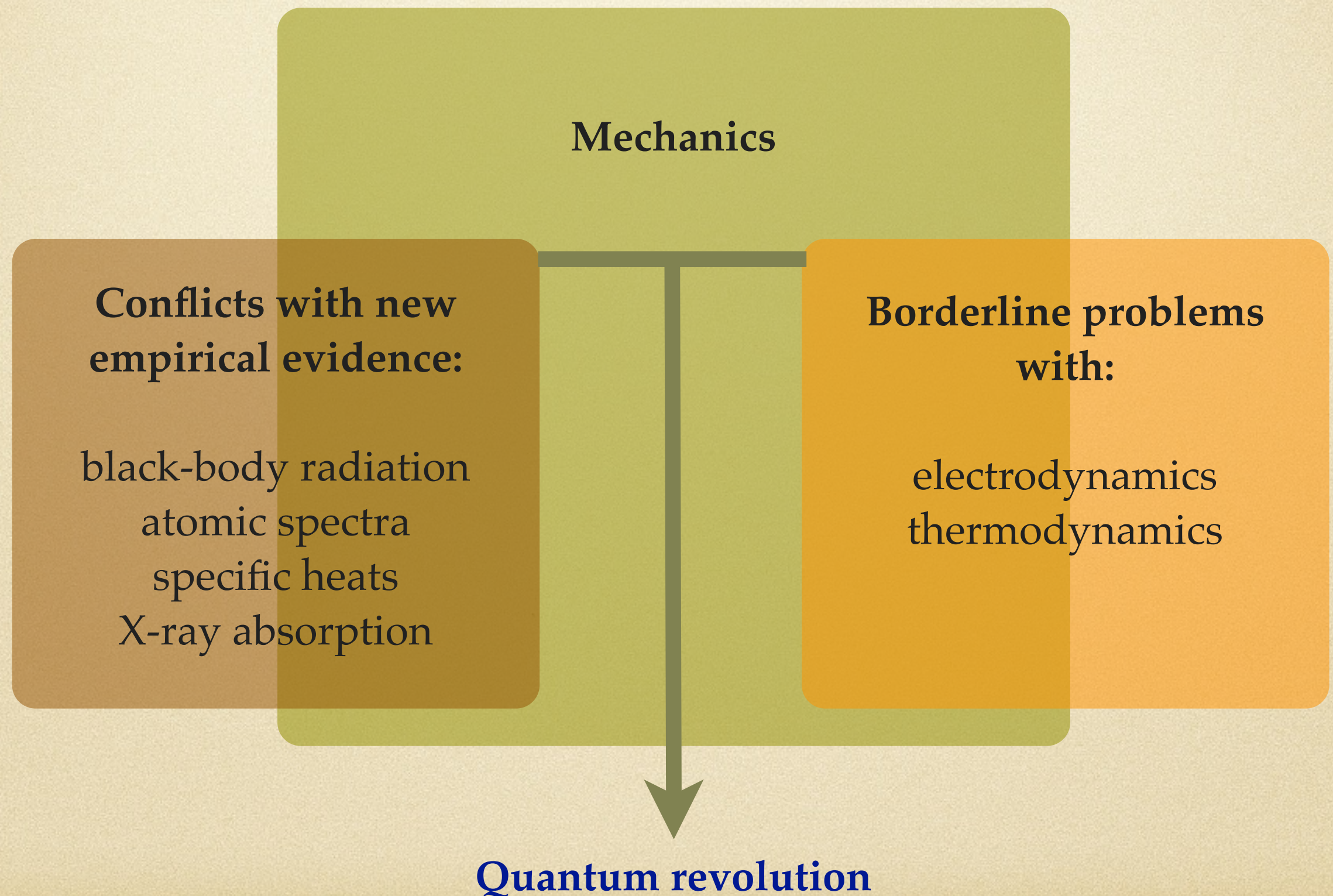
## Borderline Problems





Quantum theory and the crisis of the mechanical worldview:

## **The two-fold crisis of mechanics**





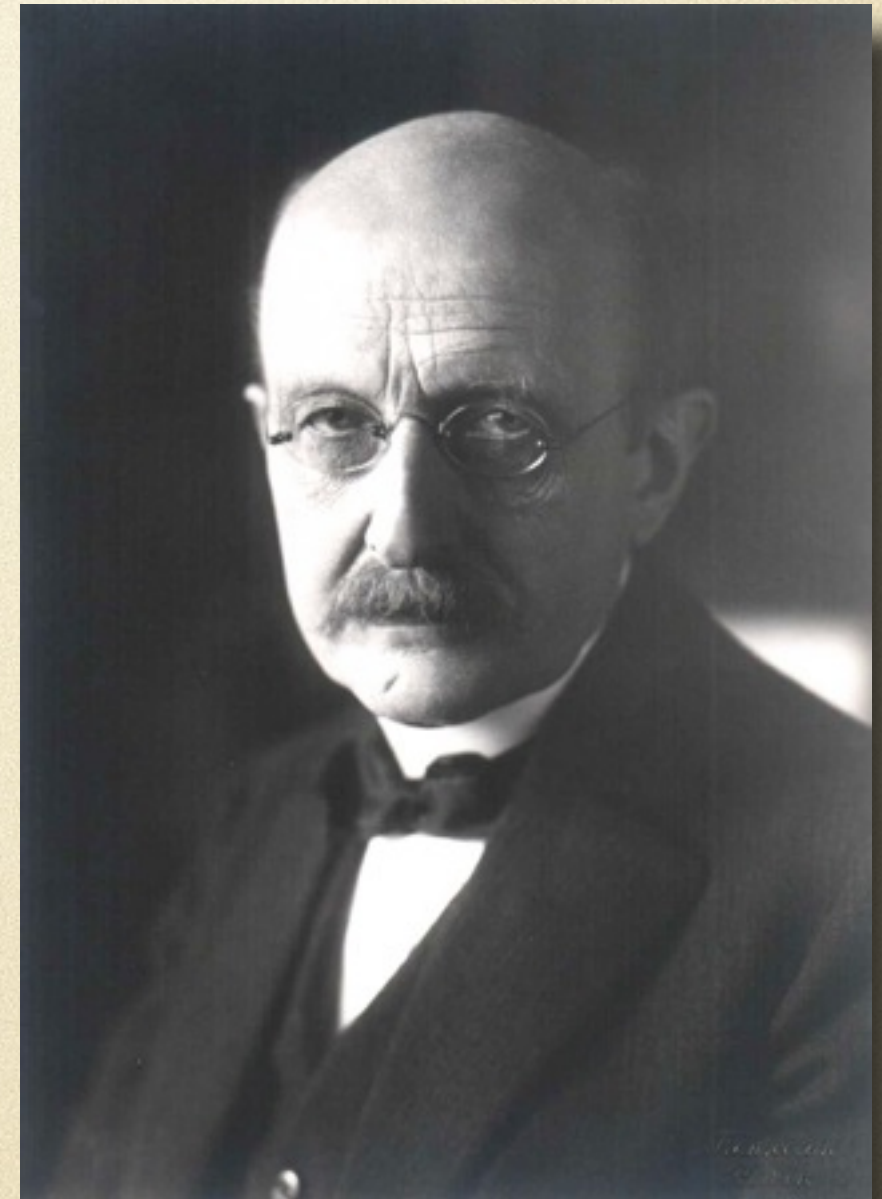
# Quantum theory and the crisis of the mechanical worldview:

## 1900: Planck's quantum hypothesis

“act of desperation”: Atoms absorb or emit energy only in elements (**quanta**) of finite size.

Leads to **black-body radiation law** describing recent empirical results:

$$\rho(\nu, T)d\nu = \frac{8\pi h\nu^3}{c^3} \frac{1}{e^{h\nu/kT} - 1} d\nu$$



Max Planck (1858–1947)



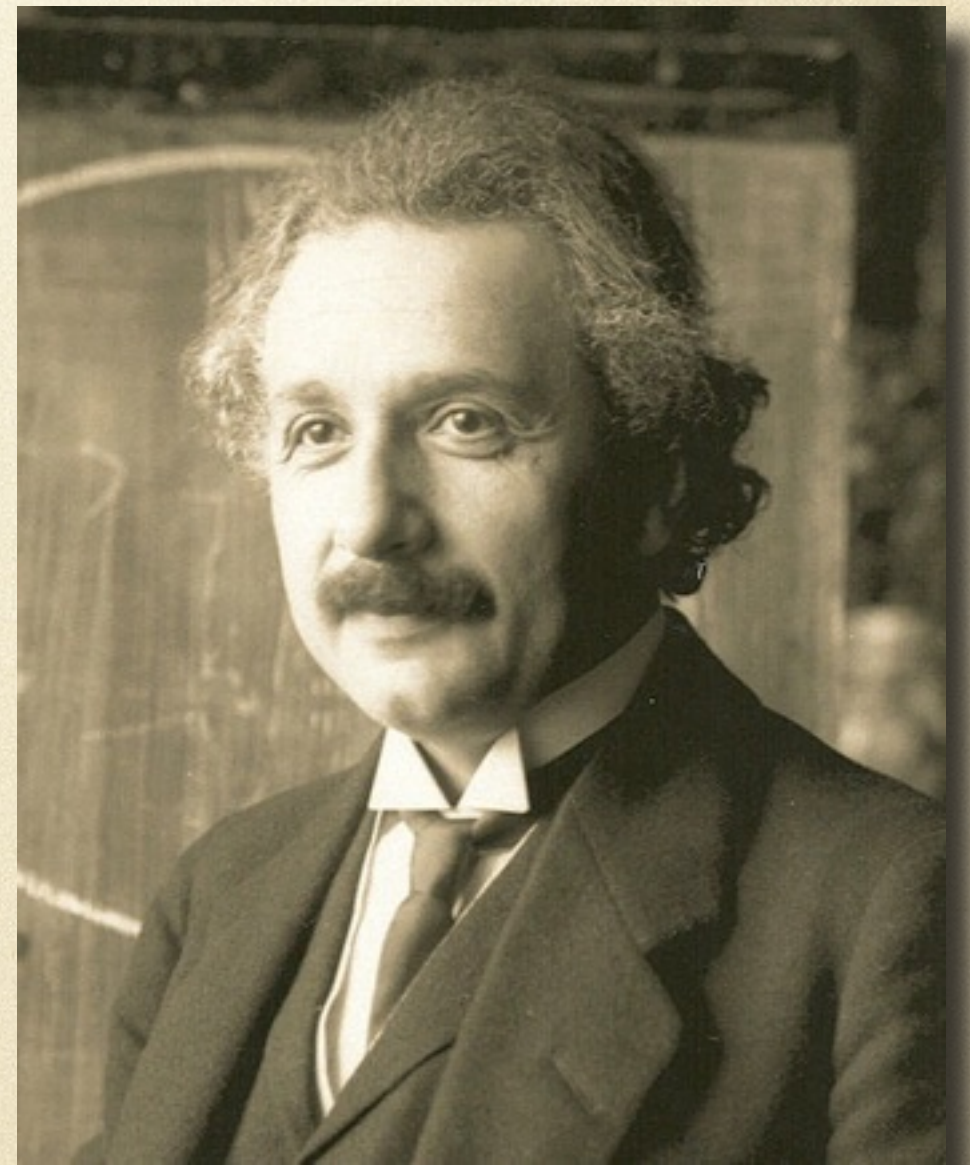
Quantum theory and the crisis of the mechanical worldview:  
**1905: Einstein's light quantum hypothesis**

Light consists of **light quanta** whose energy is given by

$$E = h\nu$$

**Highly controversial** until the early 1920s.

Leads Einstein to the idea of **wave-particle dualism of light**.



Albert Einstein (1879–1955)



Quantum theory and the crisis of the mechanical worldview:

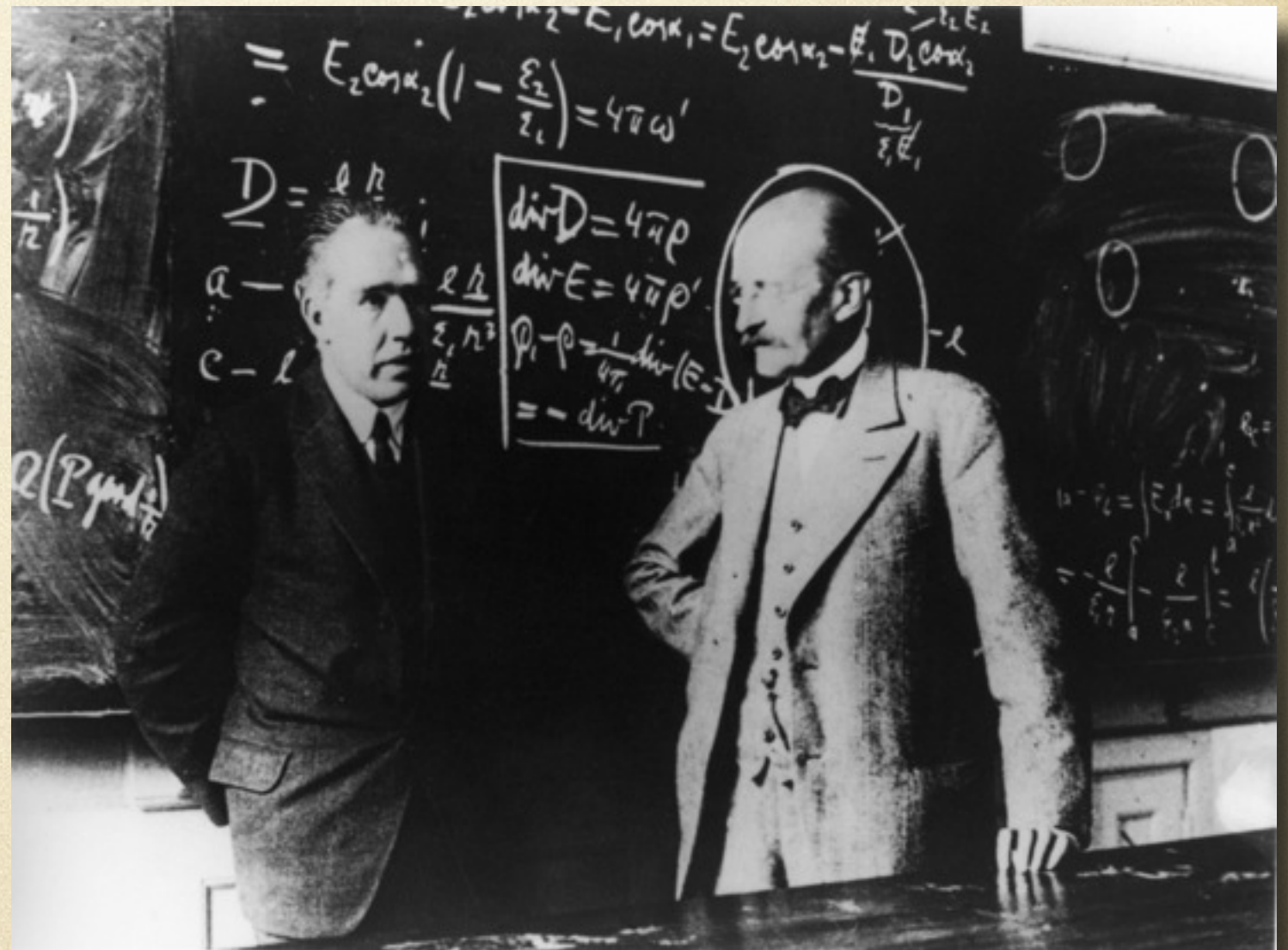
## 1913: Bohr's model of the atom

Bohr's planetary model explains hydrogen spectrum.

This leads to Bohr-Sommerfeld **quantum condition** and the so-called "old" quantum theory.

$$\oint p dq = nh$$

**Correspondence principle.**



Niels Bohr (1885–1962)

Max Planck (1858–1947)

(in Auditorium A at Copenhagen, 1930)



# Quantum theory and the crisis of the mechanical worldview:

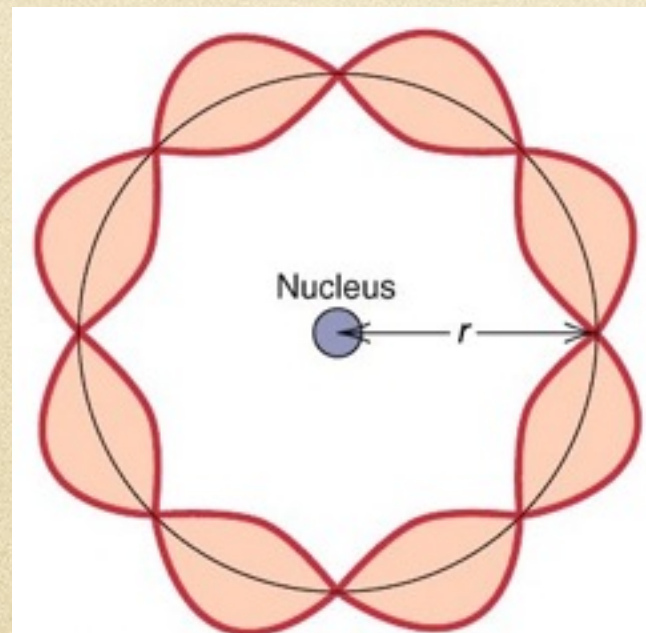
## 1924: De Broglie's matter waves

Inspired by relativity, de Broglie postulates **wave-particle duality** for light **and** matter.

**Matter waves:** “a periodic phenomenon, of a nature that remains to be determined, which is associated with every piece of matter.”

Bohr's quantum condition can be **explained** as the resonance condition for the “phase wave” along an electron orbit.

$$\lambda = \frac{h}{p}$$



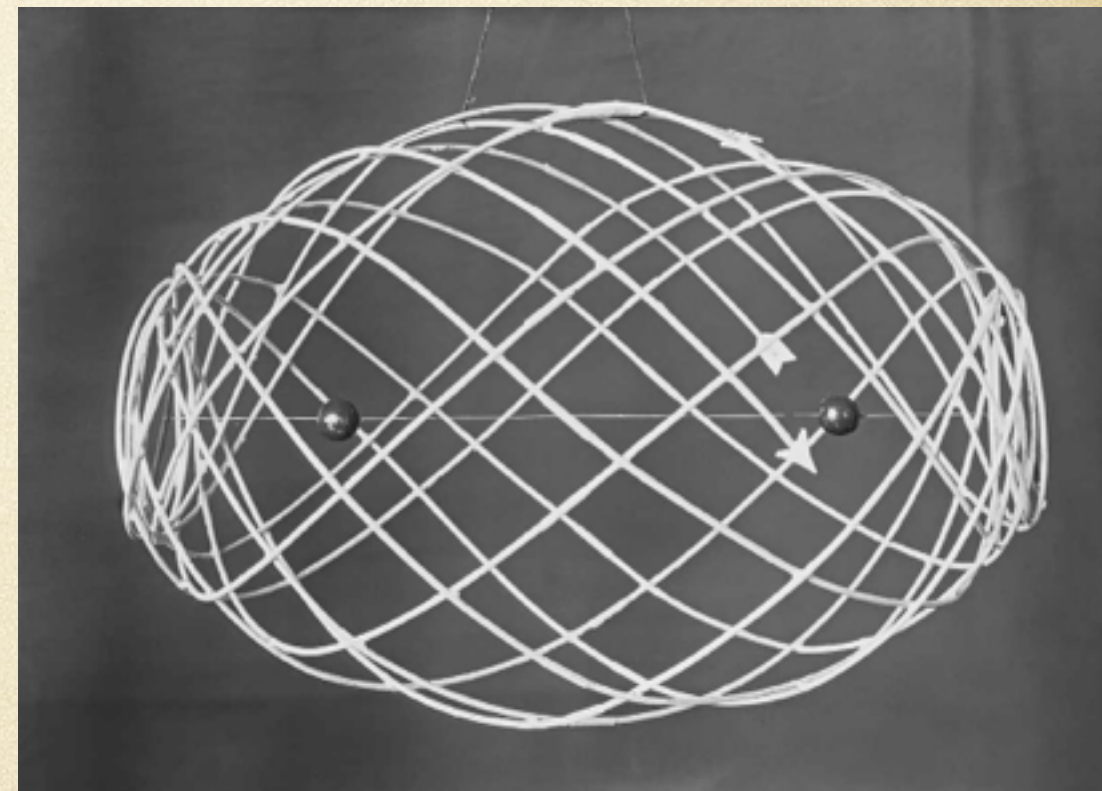
Louis de Broglie (1892–1987)



# Quantum theory and the crisis of the mechanical worldview:

## „Old“ quantum theory (ca. 1913–1925)

- More **heuristic scheme** than full-fledged theory.
- Classical mechanics “patched up” by **auxiliary** quantum conditions.
- **Fails to explain** many phenomena: Helium spectrum, Zeeman effect, multiplet structure of atomic spectra, polarization of fluorescent light, degenerate systems, aperiodic phenomena (e.g., scattering).
- From ca. 1923 on, physicists search for “**sharpened**” **formulation** of Bohr’s correspondence principle.



Model of a hydrogen molecule ion according to the old quantum theory, built for Deutsches Museum, Munich, using calculations by Wolfgang Pauli, ca. 1923.



# Quantum theory and the crisis of the mechanical worldview:

## 1925: Matrix mechanics

**Heisenberg** proposes a **new** mechanics: quantum mechanics.

“Umdeutung”: classical quantities are **reinterpreted** in terms of observable quantities, i.e., transition frequencies and amplitudes.

This amounts to a “**sharpening**” of Bohr’s correspondence principle.

**Born** and **Jordan** soon realize that Heisenberg’s involved algebra is nothing but **matrix algebra** for infinite-dimensional matrices.



Copenhagen conference (1933).  
Front row: Pauli, Jordan, Heisenberg, Born



# Quantum theory and the crisis of the mechanical worldview:

## 1926: Wave Mechanics

Based on **de Broglie's ideas** about matter waves.

Behavior of matter governed by **wave equation**

$$\Delta\psi + \frac{2m}{K^2} \left( E + \frac{e^2}{r} \right) \psi = 0$$

Astonishingly, **equivalence** with matrix mechanics is quickly established, despite the **vastly different routes** Schrödinger and Heisenberg took.



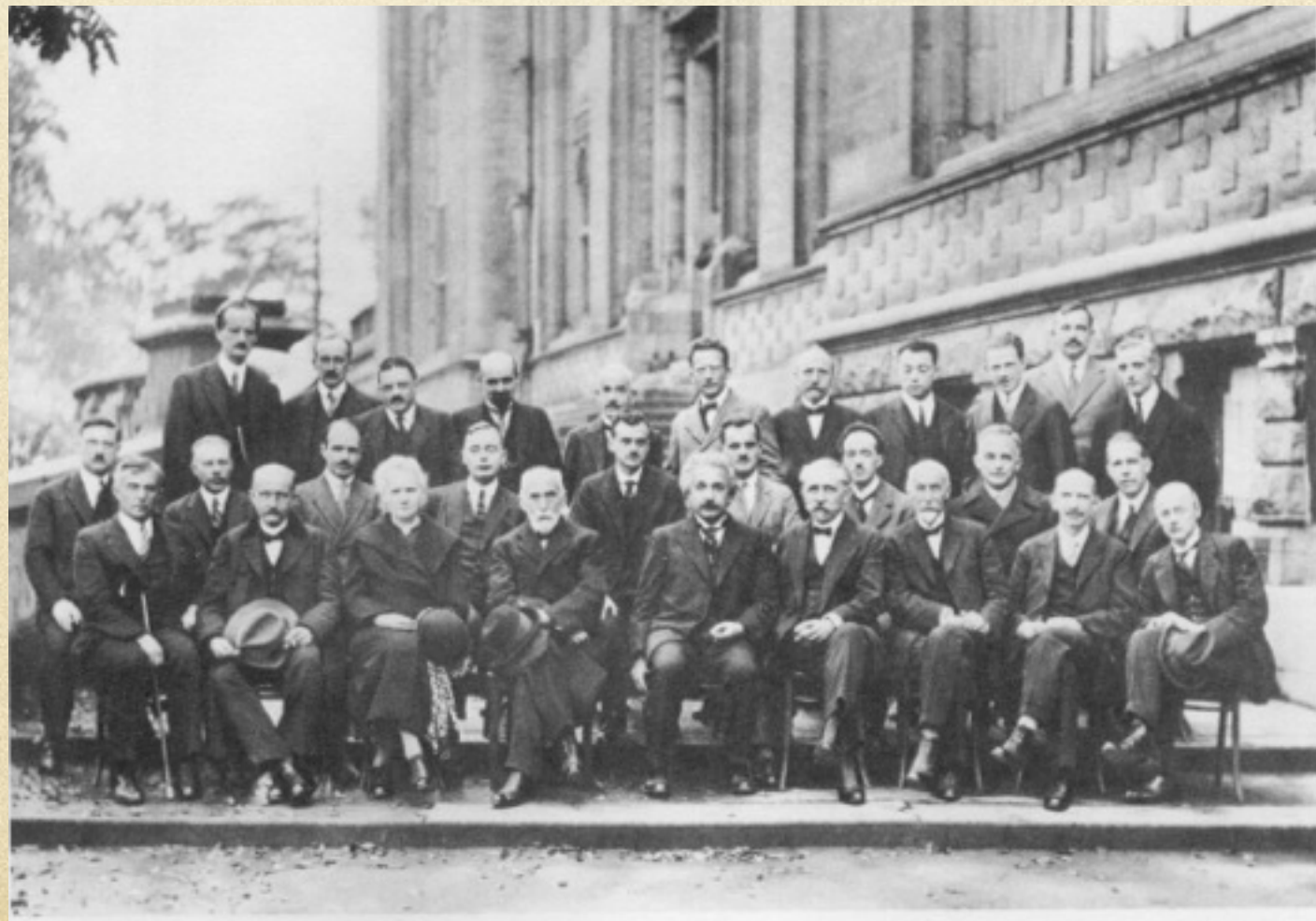
Erwin Schrödinger (1887–1961)



# Quantum theory and the crisis of the mechanical worldview:

## Further Development of Quantum Mechanics

- probability interpretation (Born) and transformation theory (Dirac, Jordan, von Neumann)
- many-body quantum mechanics (Heisenberg, Dirac, London,...)
- relativistic extension and spin (Pauli, Dirac)
- uncertainty relation (Heisenberg, Pauli)
- early quantum field theory (Jordan, Dirac)
- interpretation (Born, Schrödinger, Bohr, Heisenberg, Einstein ...)
- “applications” ...



Solvay 1927



# Quantum theory and the crisis of the mechanical worldview: **Revolution or Transformation?**

- Is the new mechanics a **wholesale replacement** or rather a **transformation** of classical physics?
- Both matrix and wave mechanics build upon **knowledge** embedded in classical physics and in the old quantum theory:
  - **Matrix mechanics:** Fourier transformations, secular perturbation theory, co-vibrations and virtual oscillators ,...
  - **Wave mechanics:** Hamilton-Jacobi theory, theory of differential equations, Hamilton's optical-mechanical analogy, ...
- Also Schrödinger's wave mechanics can be seen as a "**sharpening**" of the **correspondence principle**.

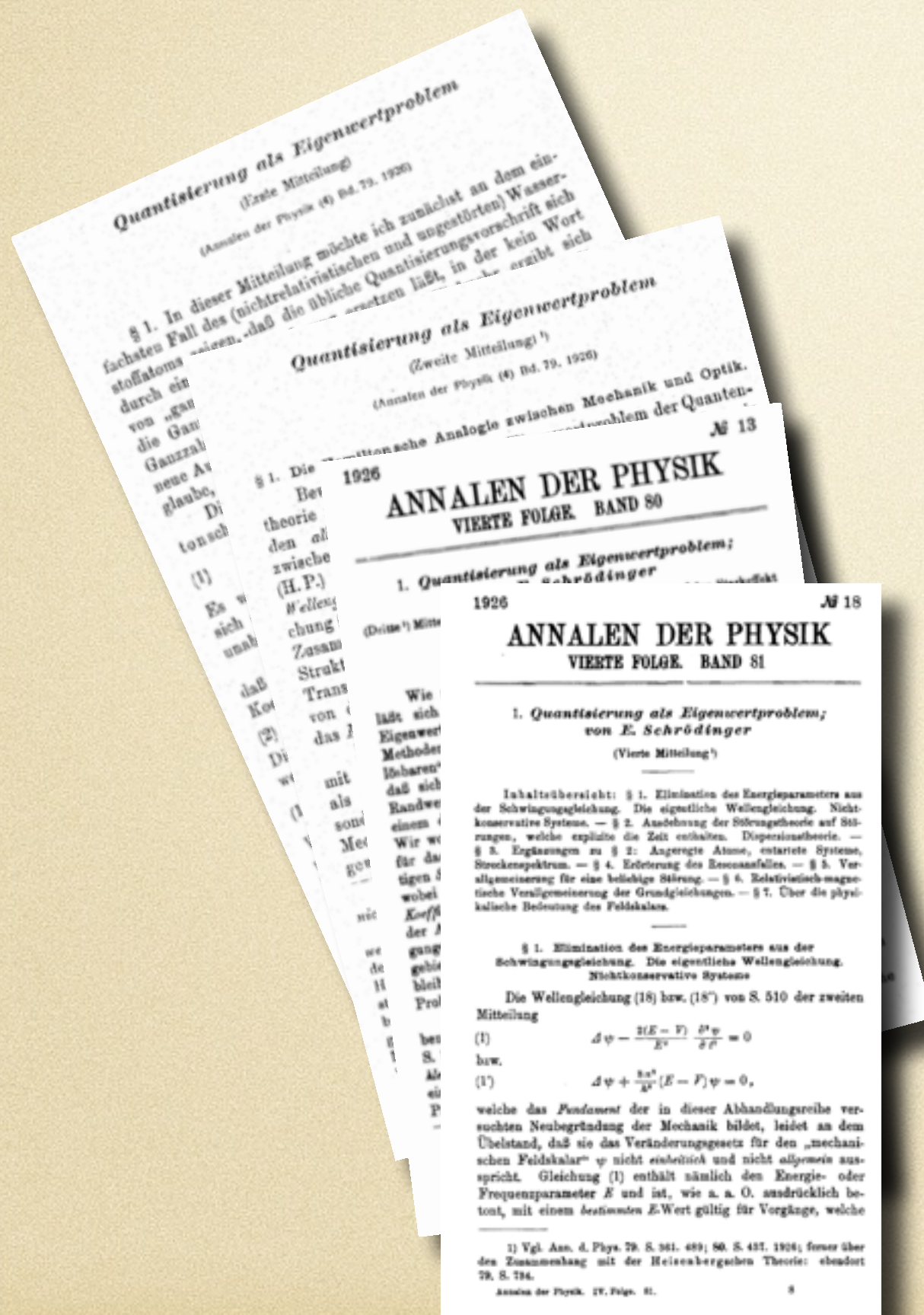


# Part II:

The genesis of wave mechanics



# The roots of wave mechanics



- 1926: Schrödinger publishes **series of four communications** in "Annalen der Physik": Quantization as an Eigenvalue Problem.
- Communications I and II present two very **different derivations** of the wave equation.
- How then **did** Schrödinger find his wave equation? What were the **roots** of wave mechanics?



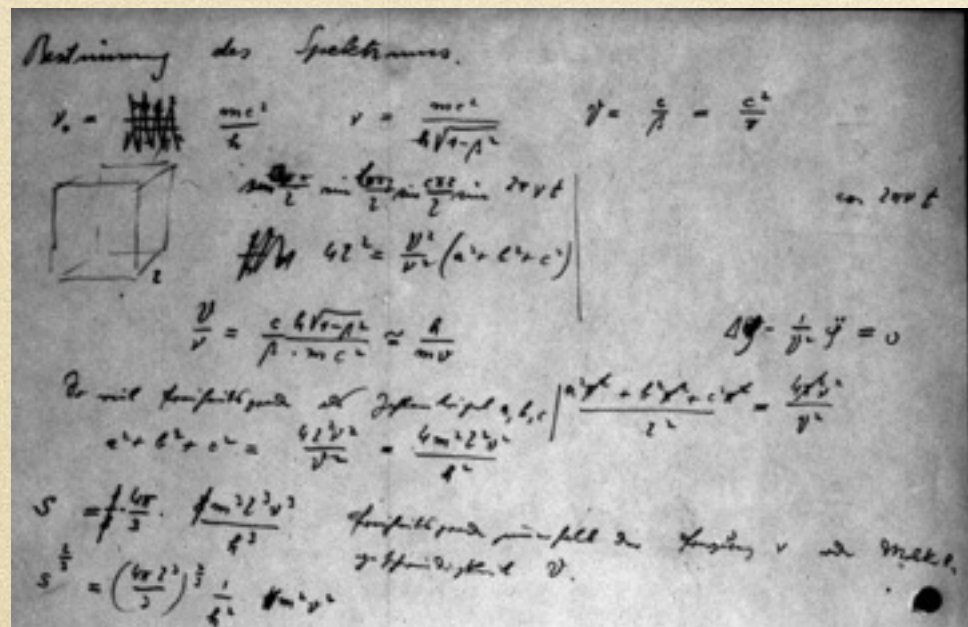
# The roots of wave mechanics

## Gas Statistics

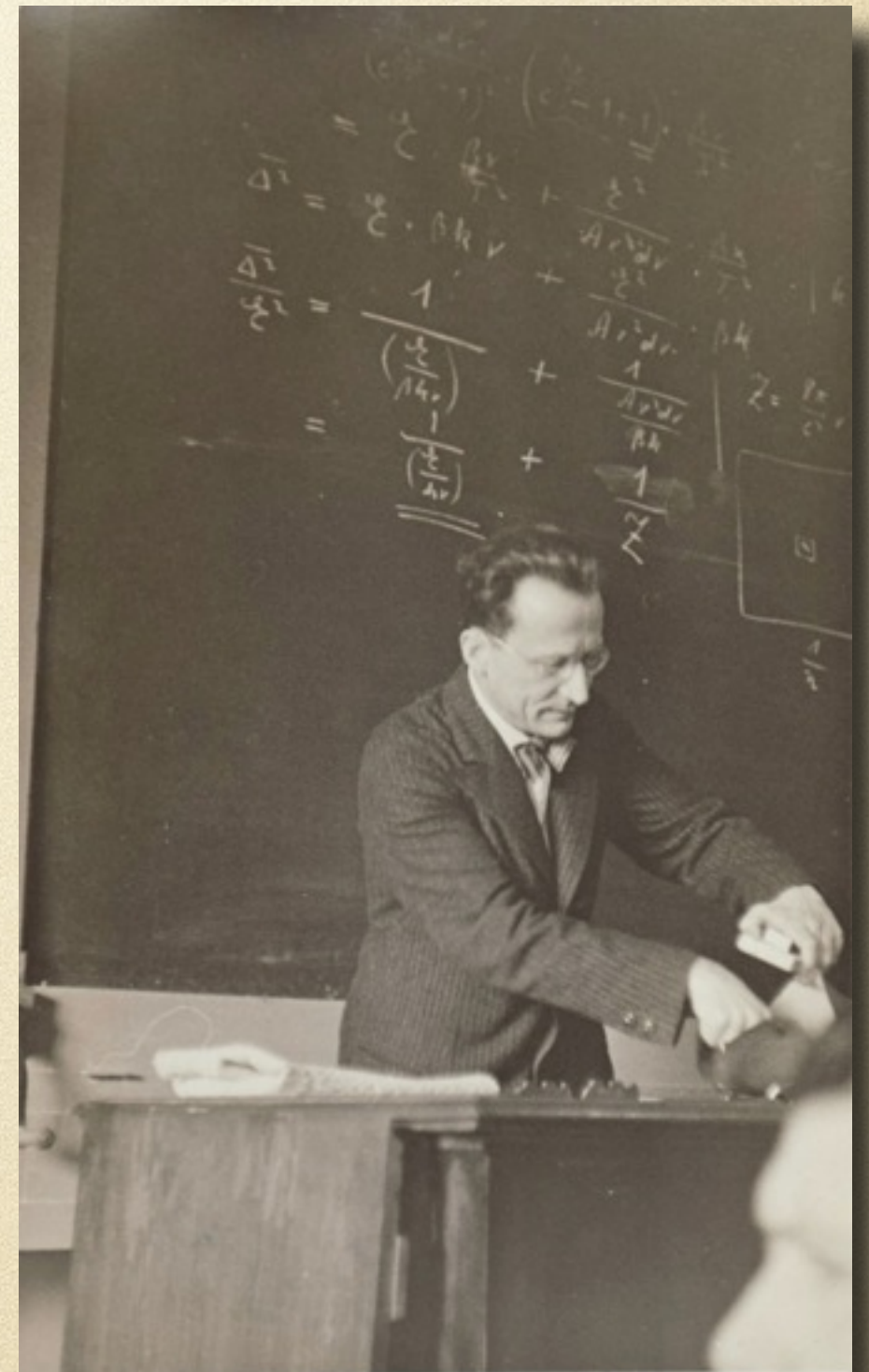
Schrödinger's central interest in 1924–1925:  
**Quantum statistics** of the ideal gas.

Schrödinger tries to make sense of the new **Bose-Einstein statistics**. Unlike his contemporaries, he is unwilling to accept the existence of a statistics **sui generis** for microscopic particles.

Through Einstein, he learns about **de Broglie** and discovers that Bose-Einstein statistics can be interpreted as a classical Boltzmann statistics of standing matter wave modes.



verso of AHQP 40-8-001 (ca. Nov. 1925)





# The roots of wave mechanics

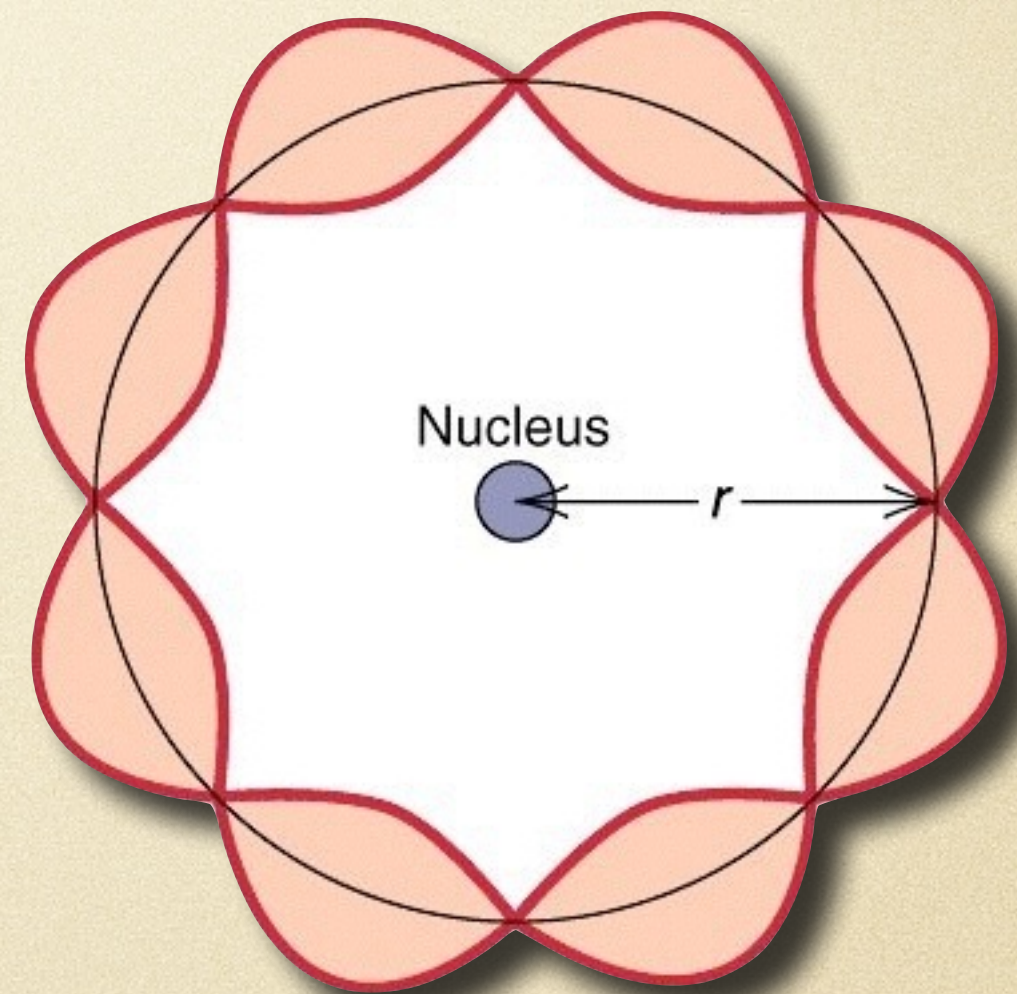
## Atomic Physics

### Alternative Explanation:

Raman and Forman (1969): Schrödinger has early interest in "**theoretical spectroscopy**," as displayed in his 1922 paper "On a Remarkable Property of Quantum Orbits of a Single Electron."

Therefore, **de Broglie**'s explanation of quantum orbits as resonance phenomenon gets picked up enthusiastically by Schrödinger.

**Problem:** Unlike in gas theory, **no evidence** for coherent research program of Schrödinger in atomic physics.





# The roots of wave mechanics

## Hamilton's Optical-Mechanical Analogy

### Third Explanation:

Helge Kragh (1982): De Broglie's use of the **optical-mechanical analogy** appeals to Schrödinger because of his own explorations of Hamiltonian mechanics around 1920. This leads him to wave mechanics.

### Problem:

Schrödinger's first communication on wave mechanics does not even mention the analogy. **It only appears in his second communication.**

This made historians like **Wessels** (1979,1983) doubt that Hamilton's analogy played a constructive role.



Sir William R. Hamilton  
(1805–1865)



# The roots of wave mechanics

## Schrödinger's research notebooks



“Schrödinger has left **few traces** of how his ideas evolved as he worked towards wave mechanics”

**Wessels** (1979)

“A considerable **mystery** now obscures the historical record. (...) The **only surviving records** from this time (...) are a three-page set of rough notes titled ‘H-Atom—Characteristic Vibrations,’ and a 72-page research notebook titled ‘Eigenvalue problem of the Atom I.’”

**Moore** (1989)

- **Both statements are wrong:** Schrödinger's notebooks provide a virtually **complete** account of the creation of wave mechanics.
- The notebooks lead to a **major revision** of previous accounts:
  - All three **roots** (gas statistics, theoretical spectroscopy, optical-mechanical analogy) have their logical place in an **ambitious research program** pursued by Schrödinger.
  - Hamilton's optical-mechanical analogy plays a **pivotal role**.



four-slide interlude:

Hamilton's optical-mechanical analogy



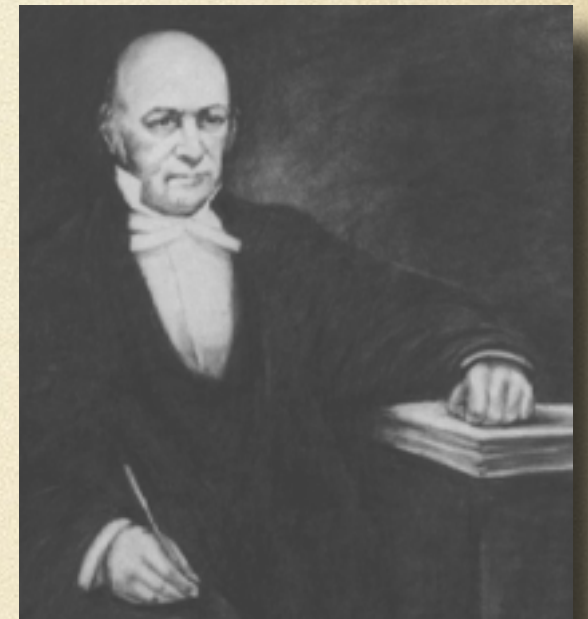
# Hamilton's optical-mechanical analogy

## Step 1: Hamiltonian optics

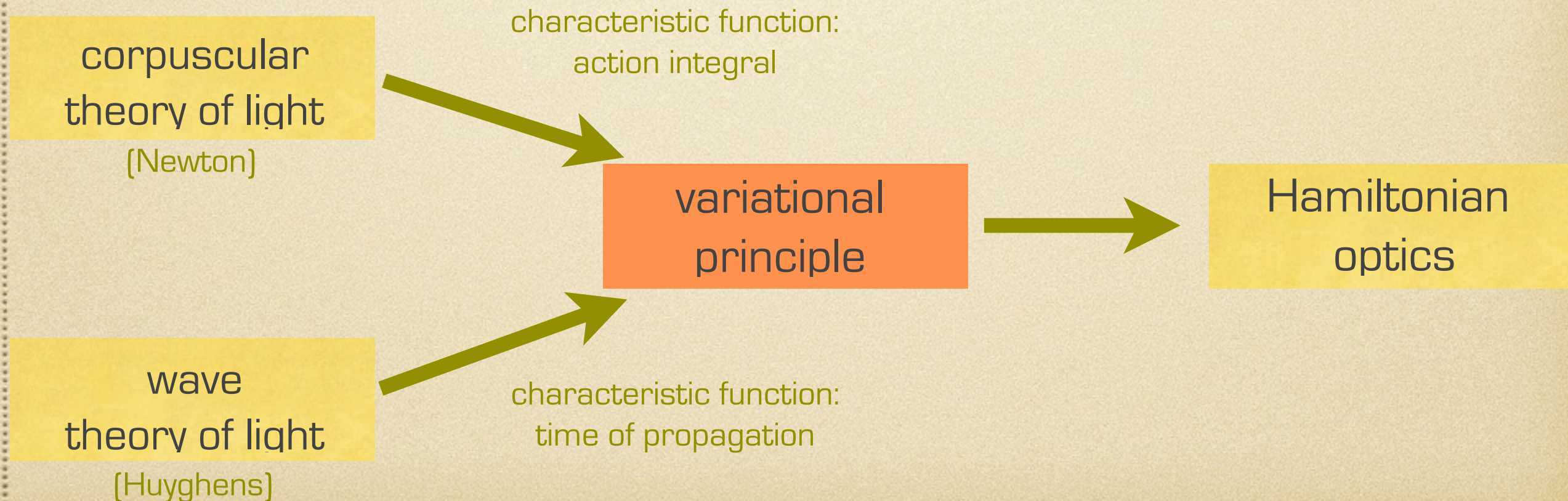
Hamilton's early work devoted to optics.

In 1833, Hamilton casts ray optics into a **general scheme** comparable to Lagrangian mechanics:

“Those who have meditated on the beauty and utility, in theoretical mechanics, of the general method of **Lagrange** [...] must feel that mathematical optics can only then attain a coordinate rank with mathematical mechanics, or with dynamical astronomy, in beauty, power, and harmony, when it shall possess an appropriate method, and become the unfolding of **a central idea**.”



Hamilton (1805–1865)





# Hamilton's optical-mechanical analogy

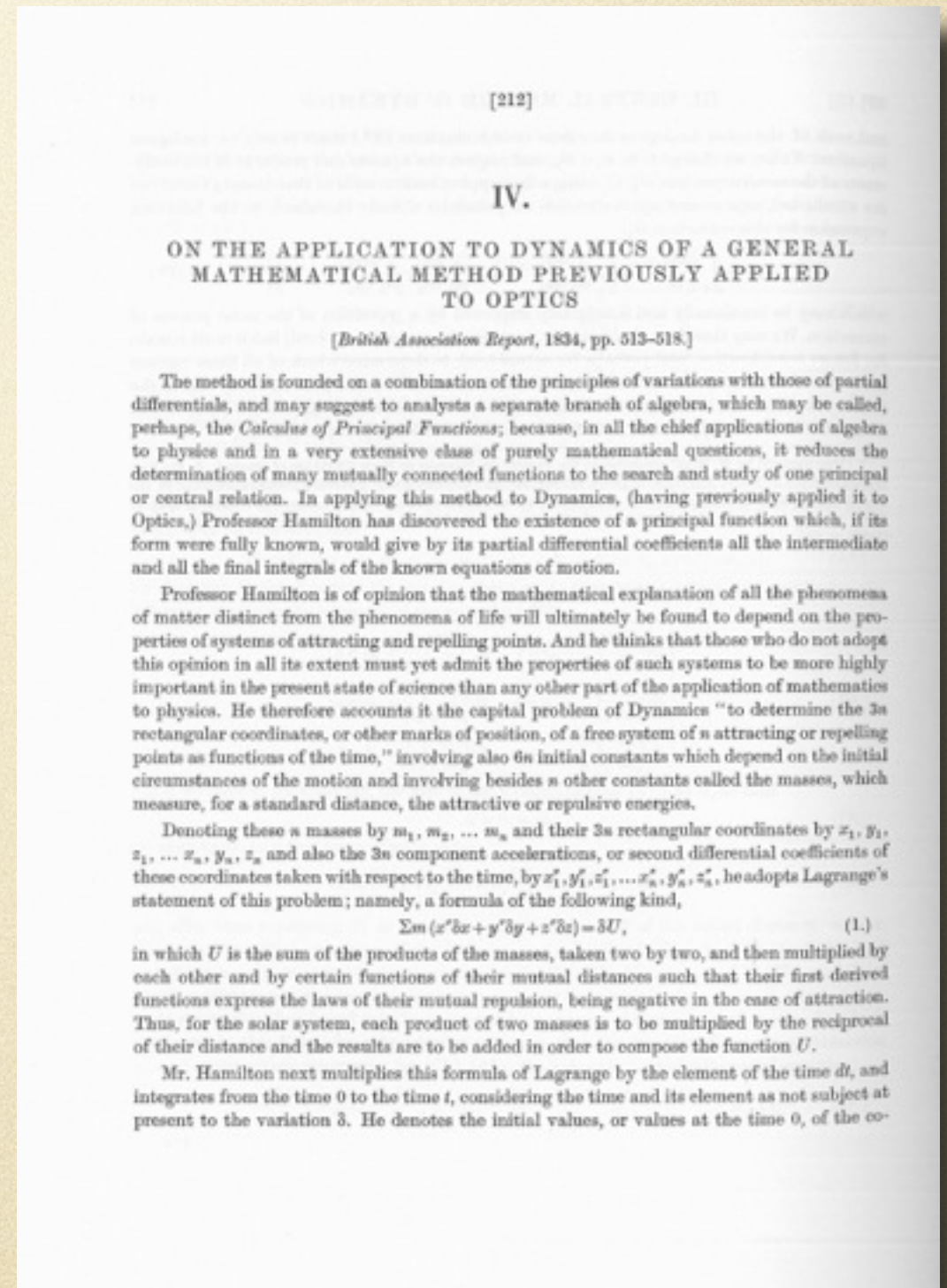
## Step 2: Unifying Optics and Mechanics

In 1834, Hamilton attempts to **unify optics and mechanics through formal analogy**.

He applies the general method he had developed for optics also to mechanics (today known as **Hamilton-Jacobi method**).

Both optics and mechanics obey a principle of least "action."

**Hamilton (1833):** "By this view the research of the most complicated orbits, in lunar, planetary, and sidereal astronomy, is reduced to the study of the properties of a single function [S]; which is **analogous to my optical function**, and represents the **action** of the system from one position to another."





# Hamilton's optical-mechanical analogy

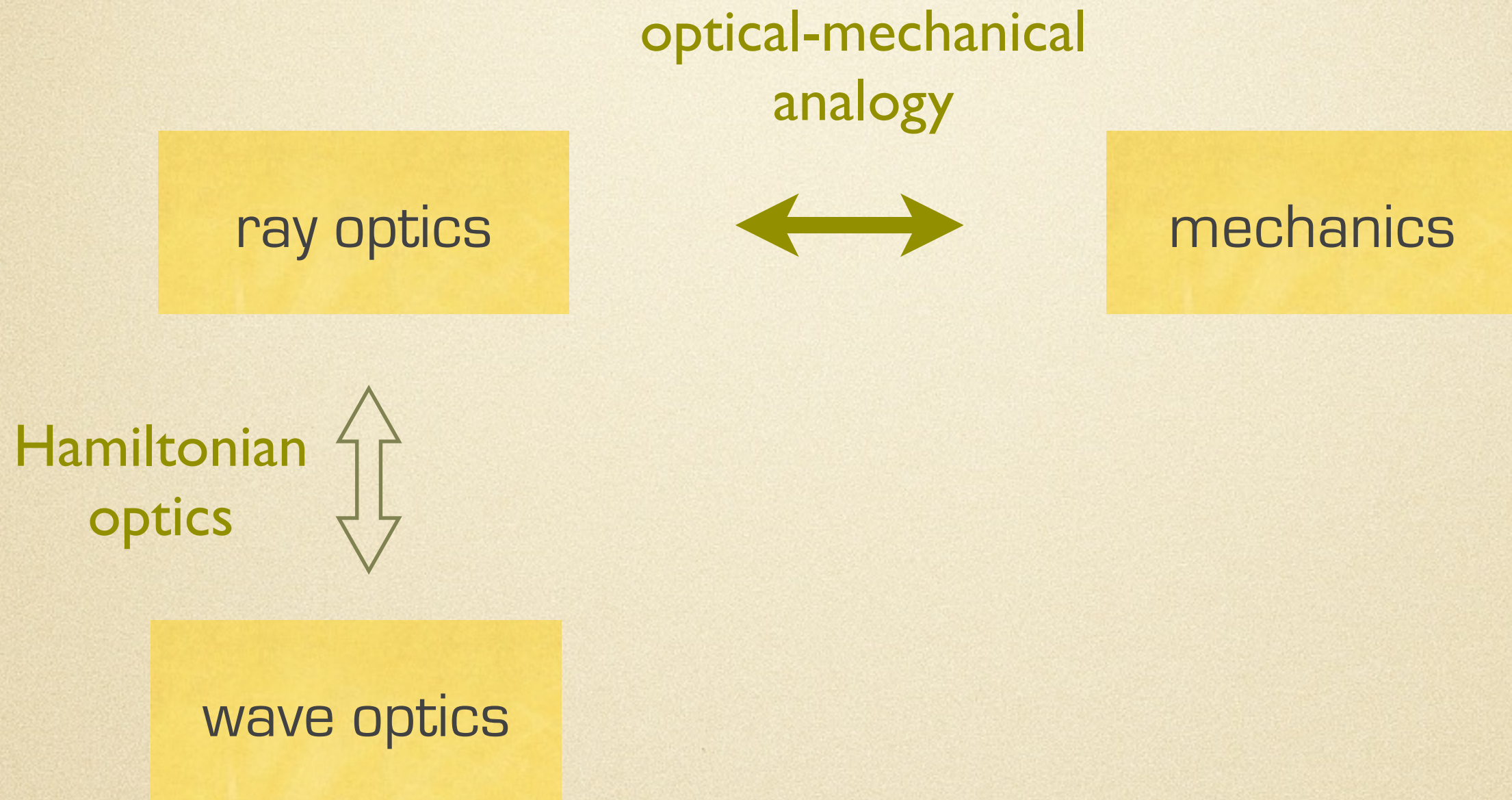
## Step 2: Unifying Optics and Mechanics

Optics:	Mechanics:
<p>Characteristic function is time of propagation <math>T</math>:</p> $T = \int \frac{n}{c} ds$ <p><math>n</math> refractive index, <math>c</math> light velocity</p>	<p>Characteristic function is action integral <math>S</math>:</p> $S = \int \sqrt{2m(E - U)} ds$ <p><math>m</math> mass, <math>E - U</math> kinetic energy</p>
<p>Integrand is inverse phase velocity <math>1/u</math>:</p> $\frac{1}{u} = \frac{n}{c}$	<p>Integrand is particle momentum <math>p</math>:</p> $p = \sqrt{2m(E - U)}$
<p><b>Fermat's principle:</b></p> $\delta T = 0$	<p><b>Maupertuis's principle:</b></p> $\delta S = 0$
<p>This implies: Light rays are orthogonal to surfaces of equal time <math>T</math> (wave fronts).</p>	<p>This implies: Particle trajectories are orthogonal to surfaces of equal action <math>S</math>.</p>



# Hamilton's optical-mechanical analogy

## Step 2: Unifying Optics and Mechanics



Until the 1920s, Hamilton's optical-mechanical analogy is nothing more than a little-known formal peculiarity.



# Part II (contd.):

The genesis of wave mechanics



# The genesis of wave mechanics

## The changing roles of Hamilton's analogy



Erwin Schrödinger (1887–1961)

- **ca. 1918–1922:** Schrödinger **encounters** the analogy when trying to generalize classical mechanics.
- **Oct–Nov 1925:** Schrödinger reads **de Broglie** in the context of gas theory and uses matter waves to explain Bose-Einstein statistics.
- **early 1926:** Analogy provides **heuristic guidance** in attempts to establish the wave equation.
- **Feb. 1926:** Schrödinger “**completes**” Hamilton’s analogy; analogy turns from heuristic tool into **formal constraint** on possible theories.
- **mid-1926:** Analogy turns into an **interpretational device**.



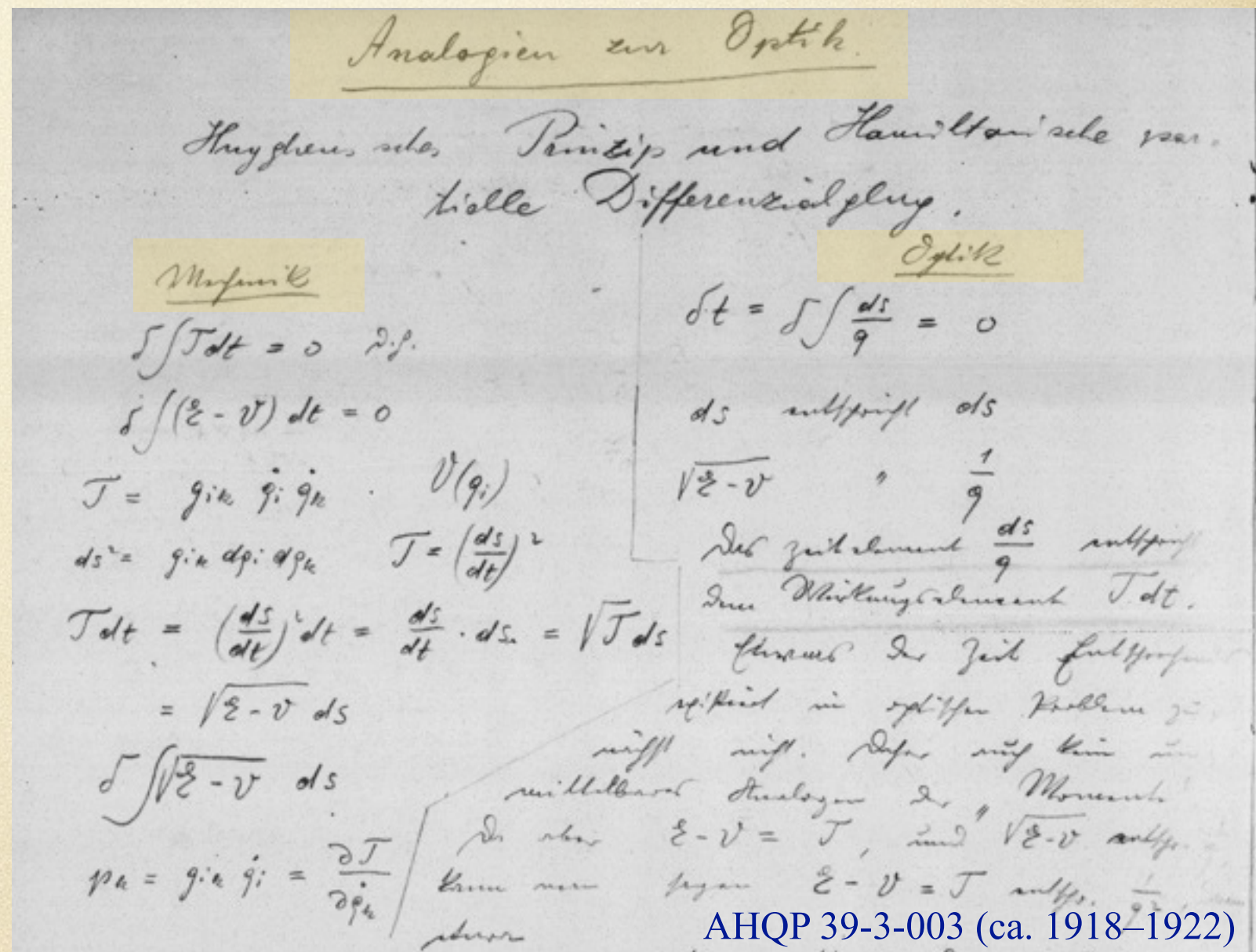
# The genesis of wave mechanics

## Schrödinger's early research program

ca. 1920: Schrödinger pursues **extensive research program** to generalize classical mechanics.

When trying to **connect** Hertzian analytical mechanics to General Relativity, he encounters the **optical-mechanical analogy**.

Schrödinger hopes that this could lead to **explanation of quantum conditions** as Hertzian constraints.



AHQP 39-3-003 (ca. 1918–1922)

Schrödinger's c. 1920 notebook on Tensor-Analytic Mechanics: working out Hamilton's analogy between mechanics (left) and optics (right).



# The genesis of wave mechanics

## Gas statistics

Physikalische Zeitschrift. 27. Jahrgang. 1926. Seite 95—101.

### Zur Einsteinschen Gastheorie.

Von E. Schrödinger.

#### § 1: Grundgedanke.

Als der wesentliche Punkt in der kürzlich von A. Einstein ausgearbeiteten neuen Gastheorie<sup>1)</sup> gilt wohl allgemein dieser, daß eine ganz neuartige Statistik, die sogenannte Bosesche Statistik<sup>2)</sup>, auf die Bewegungen der Gasmoleküle anzuwenden sei. Diese neue Statistik als etwas Primäres, nicht weiter Erklärbares anzusehen, sträubt sich das natürliche Gefühl mit Recht<sup>3)</sup>. Vielmehr scheint sich in ihr die Annahme einer gewissen Abhängigkeit voneinander oder einer Wechselwirkung der Gasmoleküle zu verhehlen, die jedoch in dieser Form nur schwer zu analysieren ist.

Man wird erwarten dürfen, einen tieferen Einblick in das eigentliche Wesen der neuen Theorie zu gewinnen, wenn es gelingt, die alten, an der Erfahrung erprobten und logisch wohl begründeten statistischen Methoden in ihrem Recht zu belassen und die Änderung in den Grundlagen an einer Stelle vorzunehmen, wo sie ohne sacrificium intellectus möglich ist. Dazu führt folgender einfacher Gedanke: die Einsteinsche Gastheorie wird erhalten, indem man auf die Gasmoleküle die Form der Statistik anwendet, die, auf die „Lichtatome“ angewendet, zum Planckschen Strahlungsgesetz führt. Aber man kann das Plancksche Strahlungsgesetz auch durch „natürliche“ Statistik gewinnen, indem man

sie auf die sog. „Ätherresonatoren“, d. i. auf die Freiheitsgrade der Strahlung anwendet<sup>4)</sup>. Die Lichtatome treten dann nur als die Energiestufen der Ätherresonatoren auf. Der Übergang von der natürlichen zur Boseschen Statistik kann stets ersetzt werden dadurch, daß man die Begriffe „Mannigfaltigkeit der energetischen Zustände“ und „Mannigfaltigkeit der Träger dieser Zustände“ die Rollen tauschen läßt. Man muß also einfach das Bild des Gases nach demjenigen Bilde der Hohlraumstrahlung formen, das noch nicht der extremen Lichtquantenvorstellung entspricht; dann wird die natürliche Statistik — etwa die bequeme Plancksche Methode der Zustandssumme — zur Einsteinschen Gastheorie führen. Das heißt nichts anderes, als Ernst machen mit der de Broglie<sup>5)</sup>-Einsteinschen<sup>6)</sup> Undulationstheorie der bewegten Korpuskel, nach welcher dieselbe nichts weiter als eine Art „Schäumkamm“ auf einer den Weltgrund bildenden Wellenstrahlung ist.

Die Durchführung dieses Gedankens scheint mir von genügendem Interesse, um sie hier auseinanderzusetzen.

#### § 2. Das Gas als Oszillatorensystem. Bestimmung der freien Energie.

Wir gehen aus von der geläufigen Vorstellung, daß jedes von den  $n$  in einem Volumen  $V$  eingeschlossenen Molekülen eines einatomigen idealen Gases eine diskrete Folge von genau

1) J. H. Jeans, Phil. Mag. 10, 91, 1905; P. Debye, Ann. d. Phys. 33, 1427, 1910. Vgl. den letzten Abschnitt von Planck, „Wärmestrahlung“. — Ferner M. v. Laue, Ann. d. Phys. (4) 44, 1197, 1914.

2) L. de Broglie, Thèse, Paris (Ed. Masson & Cie.), 1924. Gleichsam Ann. de Physique (10), 3, 22, 1925.

3) A. Einstein, l. c. § 8.

1) A. Einstein, Berl. Ber. 1924, S. 261; 1925, S. 3.  
2) Bose, Zeitschr. f. Phys. 28, 178, 1924.  
3) Vgl. A. Landé, Zeitschr. f. Phys. 33, 571, 1925.  
Im einzelnen kann ich allerdings diesen Ausführungen nicht zustimmen.



- **Oct./Nov. 1925:** Schrödinger reads **de Broglie's** thesis (letter to Einstein, 3 Nov 1925).
  - His **reinterpretation** of Bose-Einstein statistics as a “natural” Boltzmann statistics of matter waves becomes a strong argument for the correctness of the **wave picture** of matter.
- “This amounts to getting serious about the de Broglie-Einstein undulatory theory of the moving particle, according to which the latter is nothing but a kind of ‘crest’ on a wave radiation forming the substratum of the world.”



# The genesis of wave mechanics

## The relativistic wave equation

In his thesis, de Broglie refers to an analogy between **Fermat's** principle and **Maupertuis's** principle as an argument for matter waves.

Schrödinger recognizes this as an expression of the **Hamiltonian analogy**.

He introduces a tentative **relativistic wave equation** to describe de Broglie's matter waves.

Quantization rules explained as **eigenvalue problem** of a partial differential equation.

Schrödinger solves relativistic wave equation for hydrogen atom, but **fails** to derive the results of Sommerfeld's theory (**incorrect** energy levels).

Atom, Eigen schwingungen.

1.) folgendes Elektron, Dispersion der Materiewelle:

$$v = \frac{mc^2}{h\sqrt{1-\beta^2}} \quad u = \frac{c}{\beta} = \frac{c^2}{v} = \frac{\frac{mc^2}{\sqrt{1-\beta^2}}}{\frac{mv}{\sqrt{1-\beta^2}}} = \frac{|Energie|}{|Impuls|}$$

2.) Annahme Übertragung auf das Elektron im Rasterfeld:

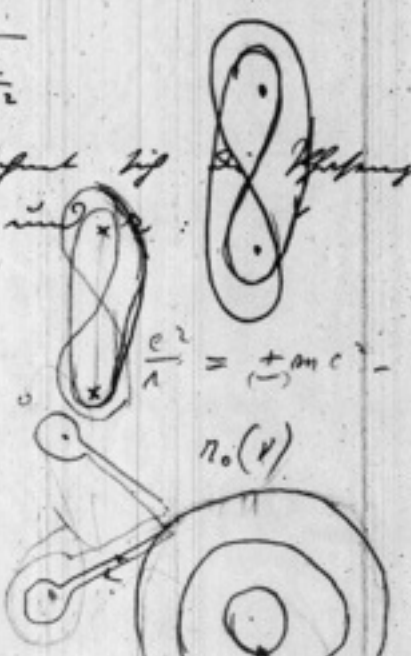
$$hv = \frac{mc^2}{\sqrt{1-\beta^2}} - \frac{c^2}{\lambda} \quad u = \frac{hv}{\frac{mv}{\sqrt{1-\beta^2}}}$$

Durch Elimination von  $v$  (oder  $\beta$ ) gelangt man zu Beziehung, die  $u$  als Funktion von  $\lambda$  liefert:

$$u = c \frac{\frac{hv}{mc^2}}{\sqrt{\left(\frac{hv}{mc^2} + \frac{c^2}{mc^2\lambda}\right)^2 - 1}} = 0 \quad \frac{c^2}{\lambda} = \frac{+mc^2}{(-)} - hv$$

mit

$$\Delta\psi = -\frac{u^2 v^2}{u^2} \psi$$

$$= -\frac{4\pi^2}{h^2} mc^2 \left( \left( \frac{hv}{mc^2} + \frac{c^2}{mc^2\lambda} \right)^2 - 1 \right) \psi$$


AHQP 40-5-002 (late 1925 or Jan. 1926)



# The genesis of wave mechanics

## The nonrelativistic wave equation (1)

In early 1926, Schrödinger derives **nonrelativistic** wave equation yielding **correct** energy levels for hydrogen atom.

Schrödinger sends off first communication in late Jan 1926, deriving nonrelativistic wave equation from seemingly **ad-hoc** variational principle.

Notebooks show: starting point is Hamilton's **optical-mechanical analogy**.

Schrödinger **reinterprets** Hamilton's equation as a field equation for the "**action field**" and uses analogy as **heuristic prescription** to convert the classical action into a picture of wave fronts.

Programm:

- 1.) Wellenmechanik des Atoms und der Lichtstrahlung.
- 2.) Die alte Hamilton'sche Analogie zwischen Optik und Mechanik.

### Program:

- 1.) relativistic treatment of the motion of the nucleus
- 2.) the old Hamiltonian analogy between optics and mechanics

$S = K \log \psi$  K Dispersions- und Mischung

$$\left(\frac{\partial \psi}{\partial x}\right)^2 + \left(\frac{\partial \psi}{\partial y}\right)^2 + \left(\frac{\partial \psi}{\partial z}\right)^2 + \frac{2m}{\hbar^2} (V - E) \psi^2 = 0 \quad (1)$$

$$\delta \int \left( \frac{1}{2} \left( \frac{\partial \psi}{\partial x} \right)^2 + \dots \right) + \frac{2m}{\hbar^2} (V - E) \psi^2 d\tau = \delta \int \left( \frac{1}{2} \frac{\partial \psi}{\partial x} \frac{\partial \psi}{\partial x} + \dots \right) + \frac{2m}{\hbar^2} (V - E) \psi \delta \psi d\tau$$

$$= 2 \int \delta \psi \frac{\partial \psi}{\partial x} d\tau - \int \delta \psi \left[ \Delta \psi + 2m(E - V) \psi \right] d\tau$$

$\frac{\partial \psi}{\partial x}$  in  $\infty$  flüchtet vor  $\frac{1}{R^2}$  von Hamilton:

$$\Delta \psi + 2m(E - V) \psi = 0$$

$\psi = -\frac{e^2}{2}$

AHQP 40-5-003  
(Jan. 1926)

Schrödinger's wave equation (almost)



# The genesis of wave mechanics

## The nonrelativistic wave equation (2)

However, for Schrödinger, it is only a **limited success**.

He turns back to the **relativistic case**, trying to improve upon the nonrelativistic wave equation for a second communication.

Starting point again:  
**Hamilton's analogy!**

fall lautet:

$$\frac{\partial S}{\partial t} + \left(\frac{\partial S}{\partial x}\right)^2 + \left(\frac{\partial S}{\partial y}\right)^2 + \left(\frac{\partial S}{\partial z}\right)^2 + V = 0 \quad (1')$$

wobei  $S$  jetzt eine Funktion von  $x, y, z$  und  $t$ .

Die Gleichung (1') erscheint jedoch über alle Verhältnisse hinweg unvollständig, da sie die Relativitätstheorie vernachlässigt. Wir gehen deshalb sofort zu dieser über, geben in obigen den Massen, welche jetzt die Ruhe Masse  $m_0$ , die Ladung  $e$  (algebraisch) und nehmen an, dass sie in einem statischen elektrischen und magnetischen Feld befinden, das durch die Potentiale  $V, A$  beschrieben wird. Die Funktionen der Punkte lautet dann bekanntlich:

$$H = m_0 c^2 \sqrt{1 + \frac{1}{m_0^2 c^2} \left[ (p_x - \frac{e}{c} A_x)^2 + (p_y - \frac{e}{c} A_y)^2 + (p_z - \frac{e}{c} A_z)^2 \right]} + e V \quad (6)$$

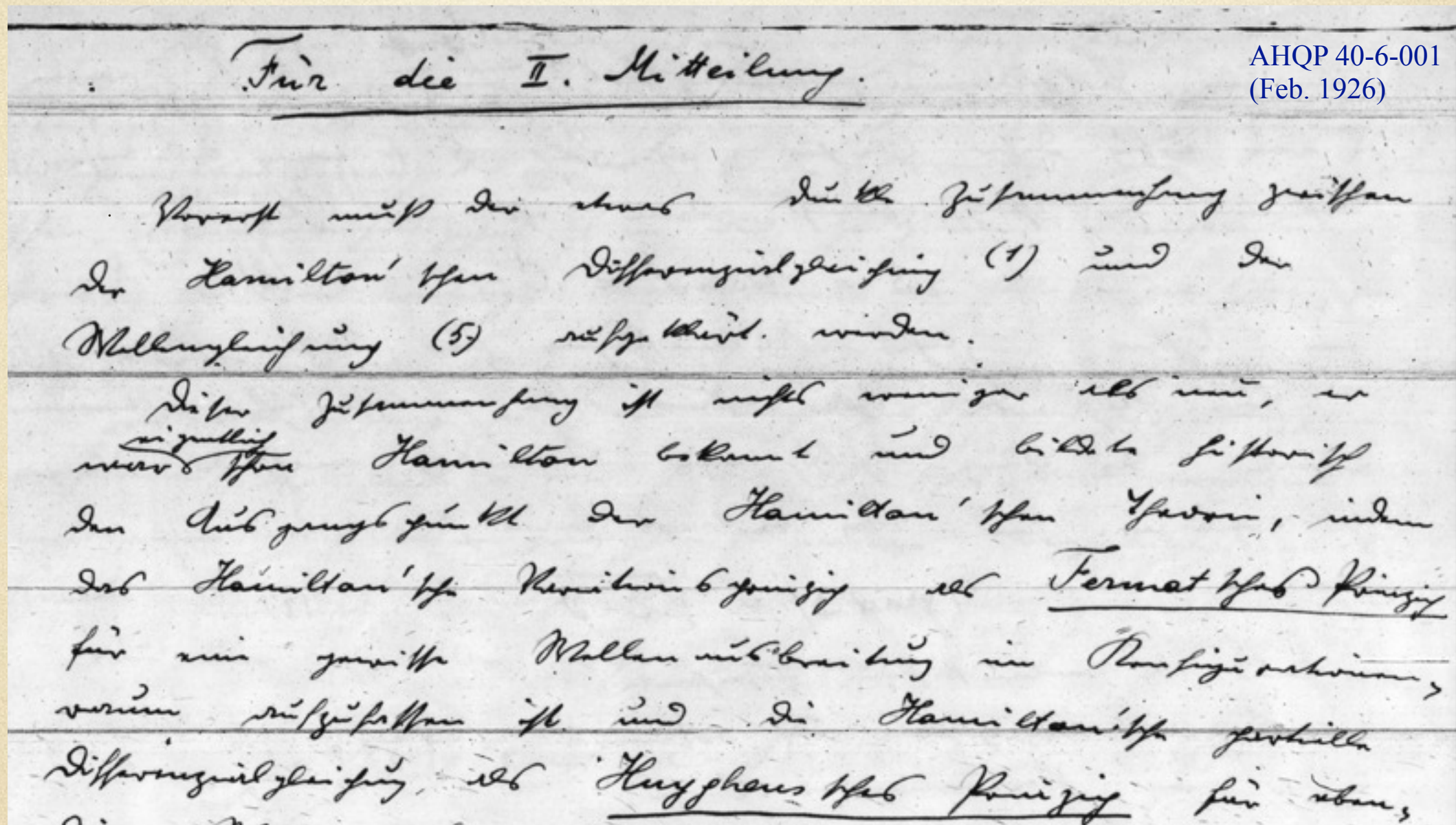
AHQP 40-6-001  
(Jan. 1926)

"The equation, however, turns out to be unsymmetrical and incomplete, it has rudimentary character due to nonapplication of the theory of relativity. Therefore, we immediately turn to [the relativistic case] ..."



# The genesis of wave mechanics

## The second communication



AHQ 40-6-001  
(Feb. 1926)

"For the second communication.

First, the somewhat obscure connection between the Hamiltonian differential equation and the wave equation needs to be explained. This connection is nothing less than new, it was actually already known to Hamilton and historically constituted the starting point for the Hamiltonian theory..."



# The genesis of wave mechanics

## An “undulatory mechanics”

**February 1926:** When preparing his second communication, Schrödinger **suddenly** realizes that Hamilton’s action function only describes the phase (and not the amplitude) of the wave fronts. If the amplitude varies, e.g., in the case of interference,  $\psi$  is not a simple function of the action.

“Maybe our classical mechanics is the **full** analog of geometrical optics, and, as such, wrong, not in agreement with reality. It fails as soon as the radii of curvature and the dimensions of the trajectory are not large anymore compared to a certain wavelength, to which one can attribute a certain reality in q-space. In that case, one has to search for ‘**undulatory mechanics**’—and the obvious way to this end is the wave-theoretical **extension** of Hamilton's picture.”

**Schrödinger** (1926, second communication)

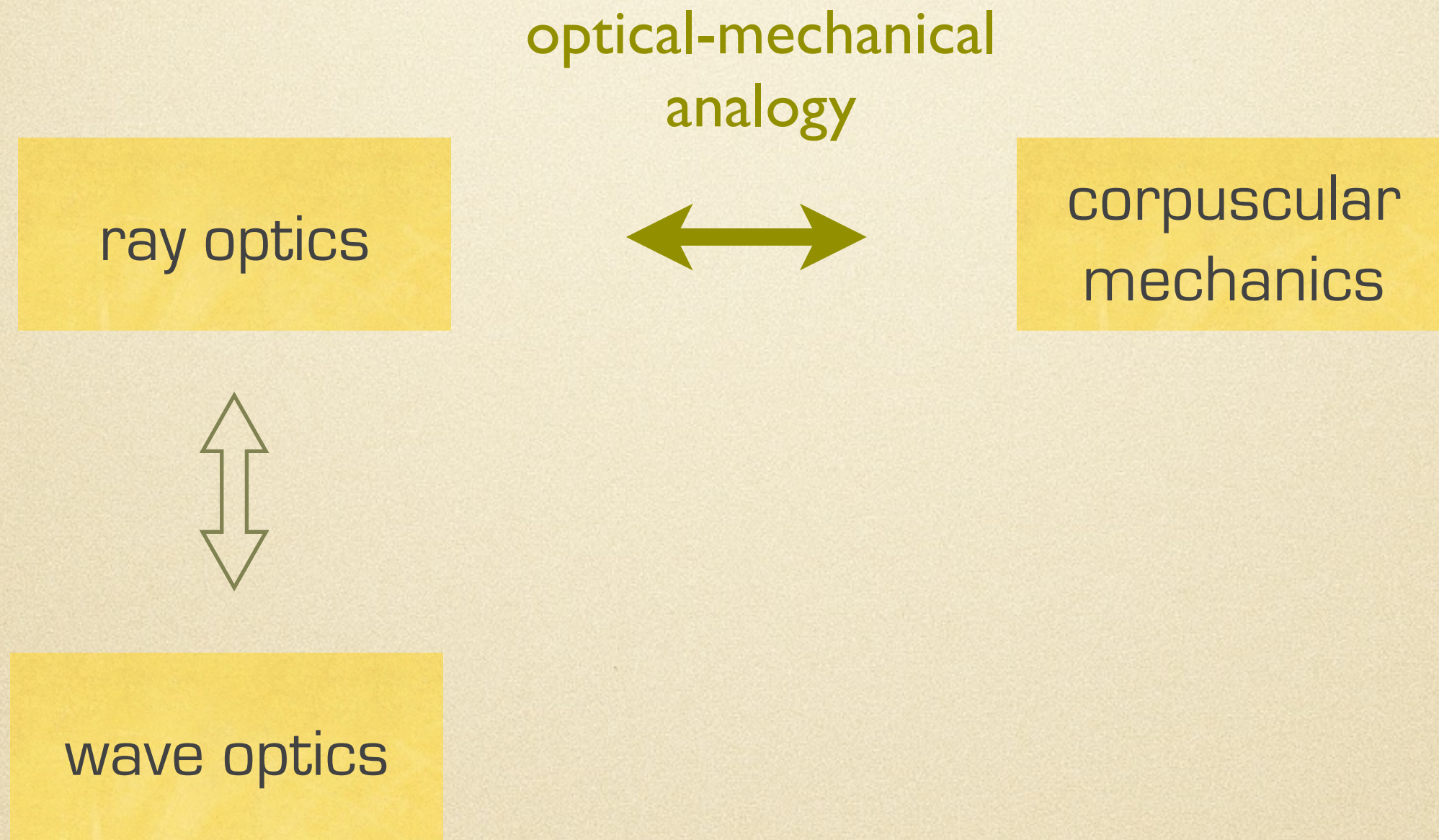


Schrödinger ca. mid-1926



# The Genesis of Wave Mechanics

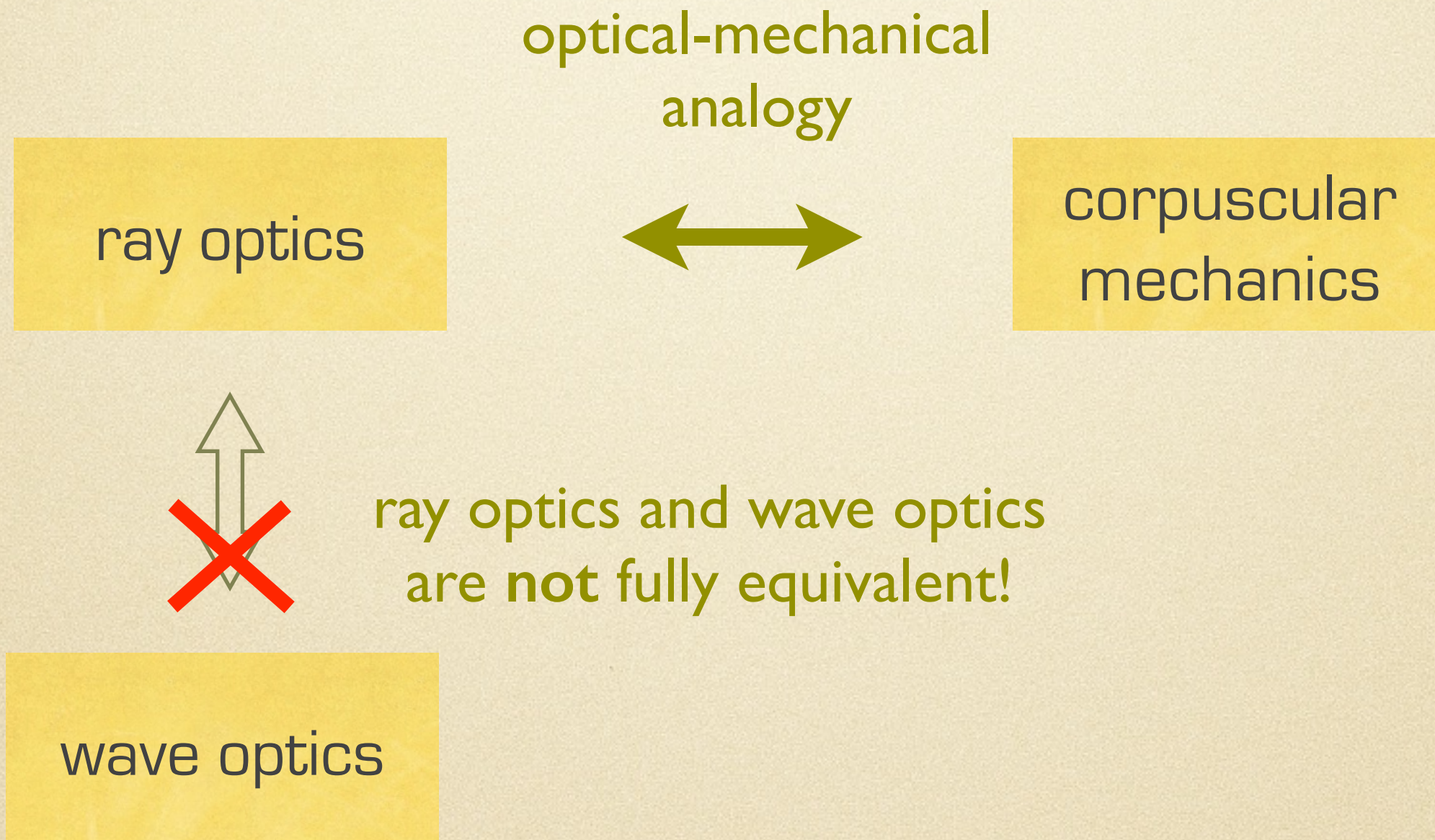
## Schrödinger's Completion of Hamilton's Analogy





# The genesis of wave mechanics

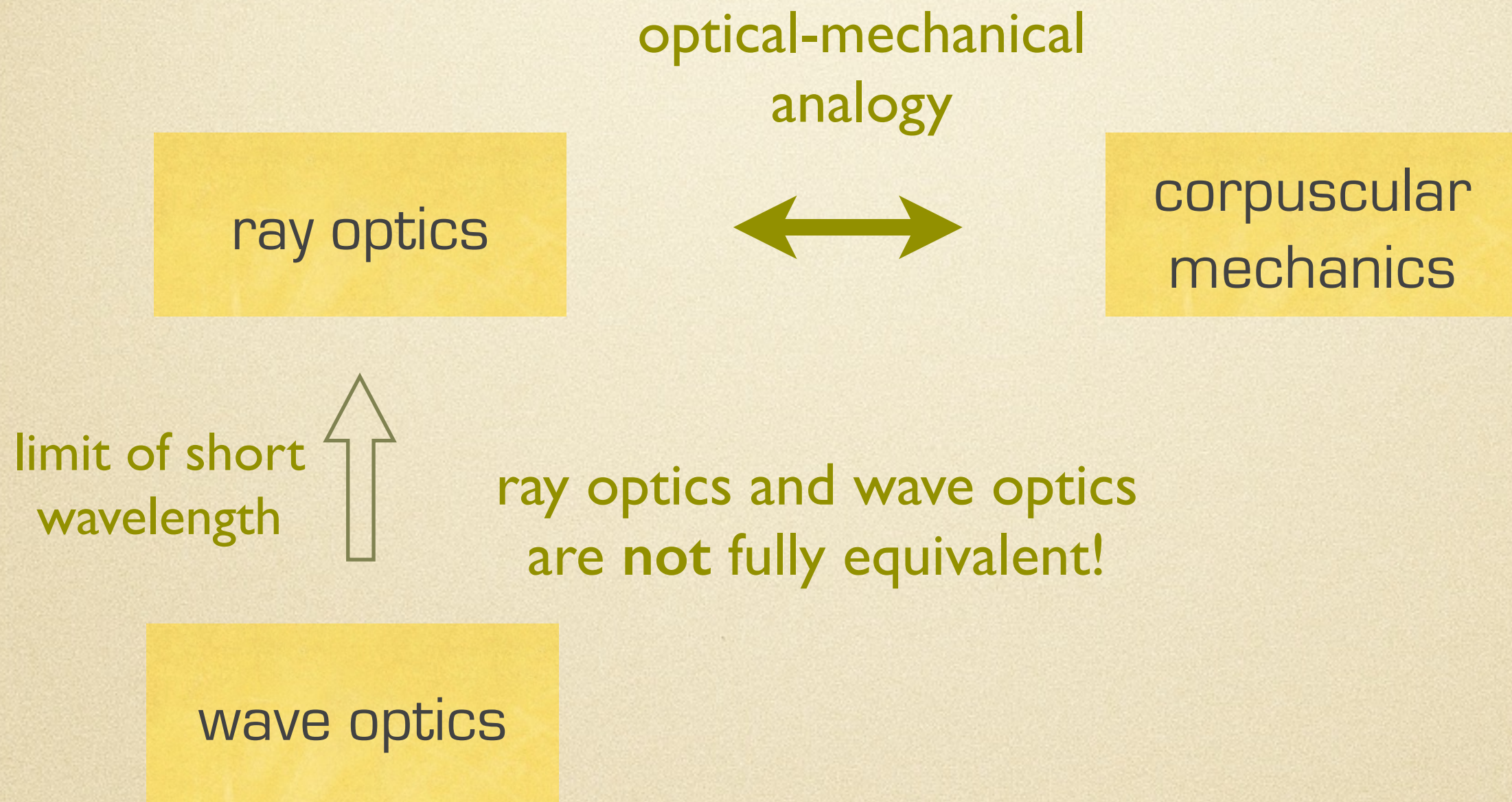
## Schrödinger's completion of Hamilton's analogy





# The genesis of wave mechanics

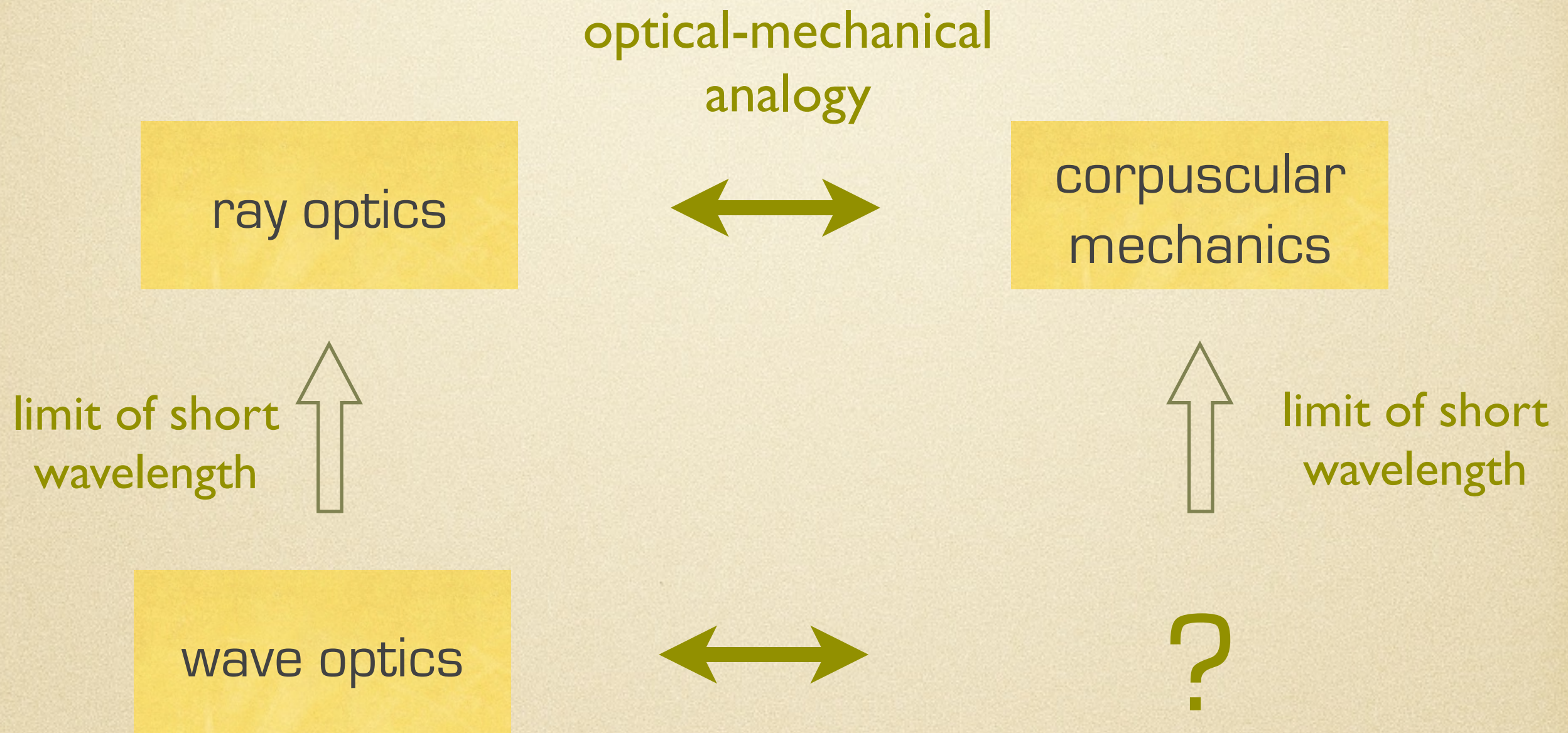
## Schrödinger's completion of Hamilton's analogy





# The genesis of wave mechanics

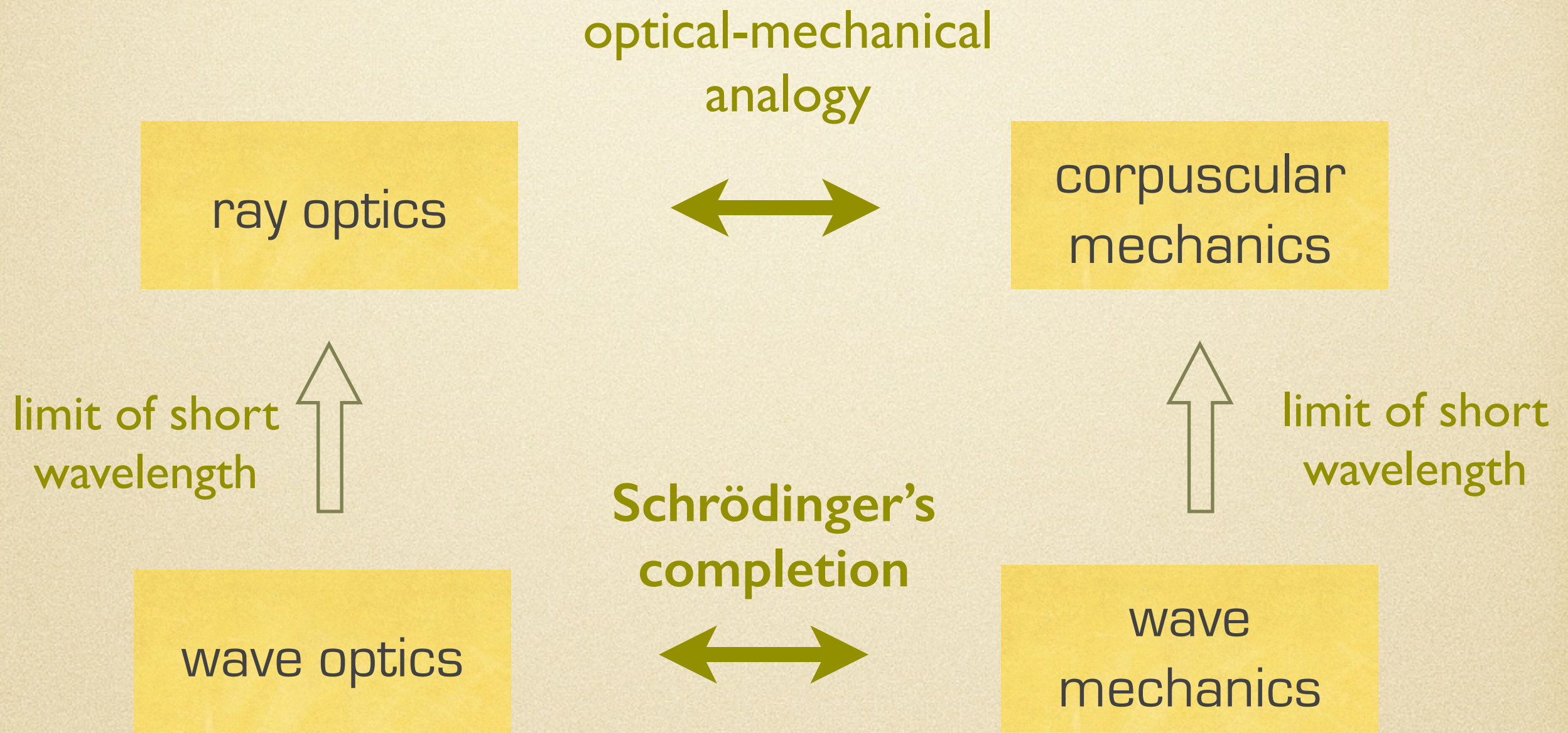
## Schrödinger's completion of Hamilton's analogy





# The genesis of wave mechanics

## Schrödinger's completion of Hamilton's analogy



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



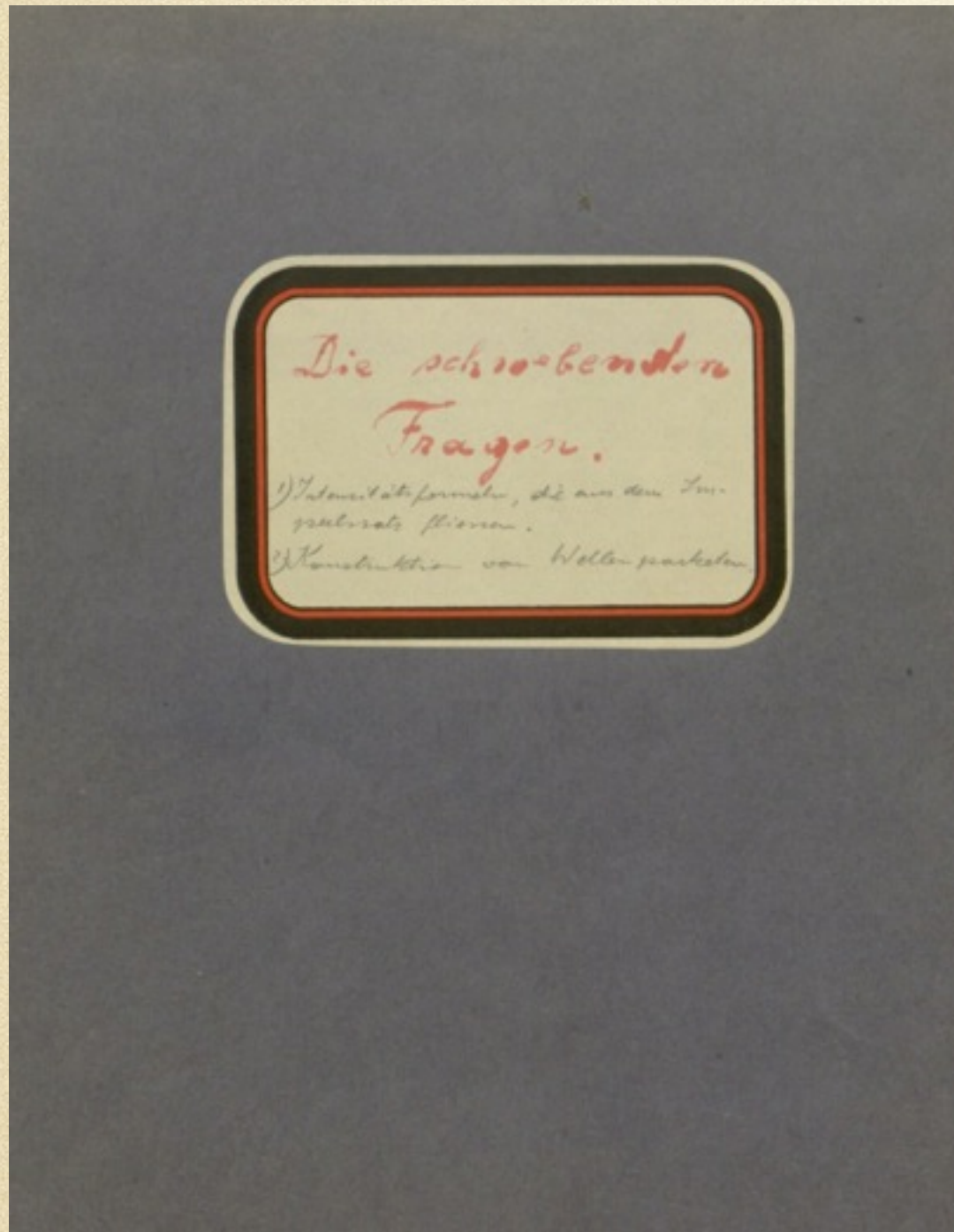
# Part III:

The "pending questions"



# Extension and Interpretation

## The Pending Questions



In the spring of 1926, Schrödinger identifies the following "**pending questions**" in his research program:

- **relation** between wave mechanics and matrix mechanics
- **relativistic extension** of wave mechanics
- **coupling** of matter field to electromagnetic field, unified field theory
- **interpretation** of the wavefunction
- **many-particle problem** within wave mechanics



# Extension and Interpretation

- During the year 1926, Schrödinger's private and public research programs begin to **diverge**.
- While focusing on successful **applications** of the nonrelativistic wave equation in his published work, Schrödinger's notebooks show him working much more intensively on **fundamental** questions of his more general program.
- He relies on the physical reading of the completed optical-mechanical analogy and searches for a "realist" **wave interpretation** of quantum mechanics.



“Baptism of the *wave packet*” (undated)



# Extension and Interpretation

## Relation to Matrix Mechanics

Schrödinger initially hopes that the optical-mechanical analogy ultimately will lead to a wave mechanics that is both **more general** (relativistic) and **heuristically more productive** than matrix mechanics.

In March 1926, he publishes "On the Relation of the Heisenberg-Born-Jordan Quantum Mechanics to Mine," (first published account of **equivalence** between matrix and wave mechanics).



unknown date and occasion



# Extension and Interpretation

## Interaction of Matter Field and Electromagnetic Field

Schrödinger keeps searching for the **relativistic generalization** of the wave equation. His attempts get ever more desperate.

A central question becomes the problem of formulating the **coupling** of the matter field to the electromagnetic field, e.g., to explain the Zeeman effect.

Neuer Versuch das Hamiltonsche Prinzip aufzustellen.

$$-d \int \psi^2 d\tau = 1 \quad -\mu \int \Phi^2 d\tau = \text{const}$$

$$\delta J = \delta \int \left( \text{grad } \psi - \frac{2\pi e}{hc} \psi \Phi \right)^2 d\tau = 0$$

$$\begin{aligned} \frac{1}{2} \delta J &= \int \left( \text{grad } \psi - \frac{2\pi e}{hc} \psi \Phi \right) \left( \text{grad } \delta \psi - \frac{2\pi e}{hc} \Phi \delta \psi - \frac{2\pi e}{hc} \psi \delta \Phi \right) d\tau \\ &= \int \left[ \text{grad } \psi \cdot \text{grad } \delta \psi - \frac{2\pi e}{hc} \psi \left( \Phi \text{grad } \delta \psi \right) - \frac{2\pi e}{hc} \Phi \text{grad } \psi \cdot \delta \psi + \right. \\ &\quad \left. + \frac{4\pi^2 e^2}{h^2 c^2} \Phi^2 \psi \delta \psi - \frac{2\pi e}{hc} \psi \text{grad } \psi \delta \Phi + \frac{4\pi^2 e^2}{h^2 c^2} \psi^2 \Phi \delta \Phi \right. \\ &\quad \left. - \frac{1}{2} \delta \psi^2 - \mu \Phi \delta \Phi \right] d\tau \end{aligned}$$

Wupin. So kann es nicht gehen.

Rot  $\Phi$  muss kommen. Das Feld.

“New attempt to formulate Hamilton’s principle” [including the interaction between the matter field and the electromagnetic field]



# Extension and Interpretation

## Interpretation of the Wave Function

Kann man  $\psi \frac{\partial \psi}{\partial t}$  als Dichte berechnen?

Das Dichte darf nur eine Größe bezeichnet werden, welche mindestens folgendes 2. Ansehen genügt

1.) Die mit  $\psi$  verknüpfte Bewegung muss einer Lawe-Mechanik unterworfen werden können.

2.)  $\psi$  muss wenigstens ein Hamiltonintegral zulässig kuppeln sein, und auch die Bewegungsgleichung  $\frac{d\psi}{dt}$  erfüllbar ist.

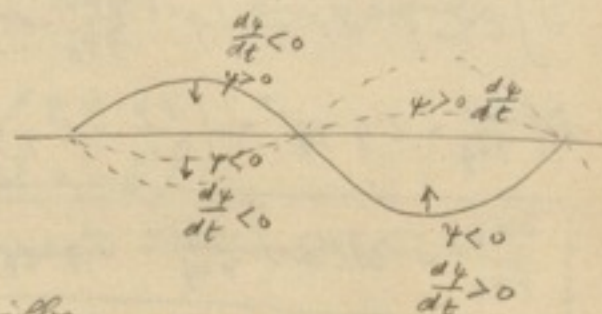
Will 2.) von  $\psi \frac{\partial \psi}{\partial t}$ ?

$$\int \rho(x) \psi \frac{\partial \psi}{\partial t} dx =$$

$\psi$  in ganzen Raum gleichmäßig  
und erfüllt in ganzen Raum  
periodisch der Zeit. d.h.  $\frac{d\psi}{dt}$  in berechnen.  
Sagen wir nicht

$$\psi \frac{\partial \psi}{\partial t} + \bar{\psi} \frac{\partial \psi}{\partial t}$$

gleichfalls die Funktion 2., als möglich, wie man sich leicht  
überzeugt, 0 über den ganzen Raum.



The problem of the coupling leads Schrödinger to ponder the question of the **physical meaning** of the wave function.

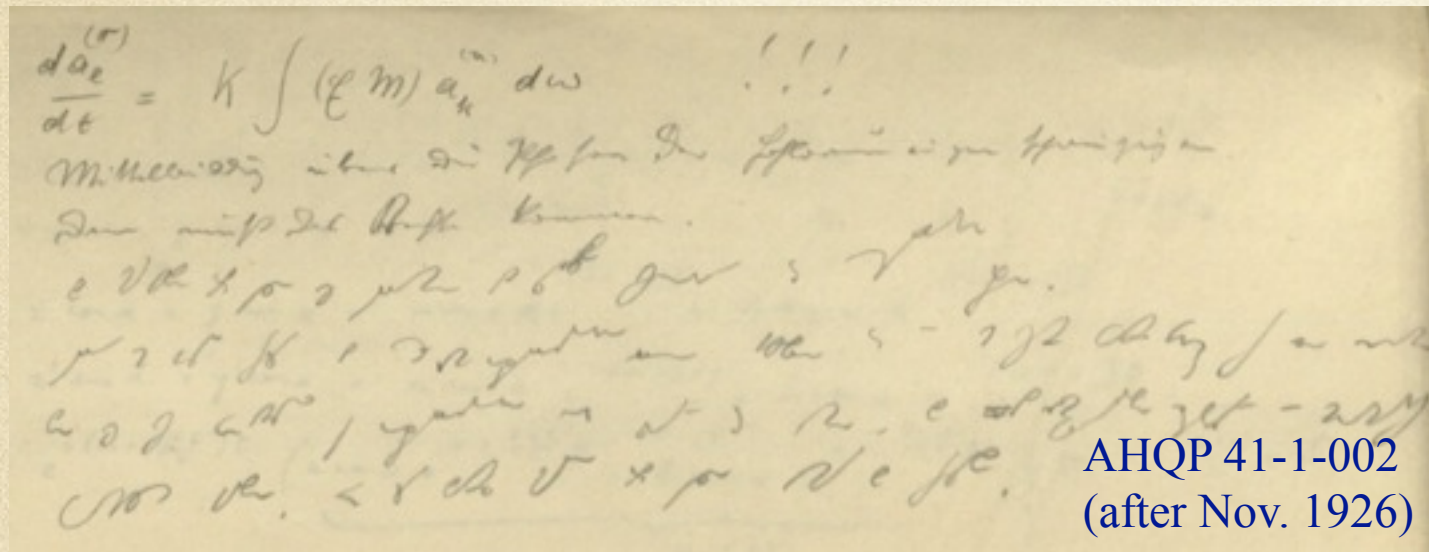
The notebooks show numerous attempts at deriving a **charge-current density** from the wave function, interpreting it as a physical wave.

In the meantime, Born proposes his **probabilistic interpretation** of the wave function. Schrödinger objects vehemently—the **interpretation debate** begins.

AHQP 41-4-001  
(Spring 1926)



# Interpretation of the Wave Function



AHQP 41-1-002  
(after Nov. 1926)

pack.18, n.4 (Einlageblatt)  
Stenogrammübertragung

Das Mittelbilden über die Phasen muß vollkommen die statistische Schweinerei aus Göttingen ersetzen.

Vielleicht am besten zuerst die Hohlraumoszillatoren allein behandeln und ganz schwache Wechselwirkung zu ihnen annehmen,

dann muß schon wenigstens für die Oszillatoren einer Sorte heraus= kommen, daß die Amplitudenquadrate eine geometrische

Progression bilden. Aber erst durch das Mitteln über die Phasen kommt das zustande.

A.D. Jan. 1931

Shorthand transcription:

"Averaging over the phases has to replace completely the Göttingen obscenity."



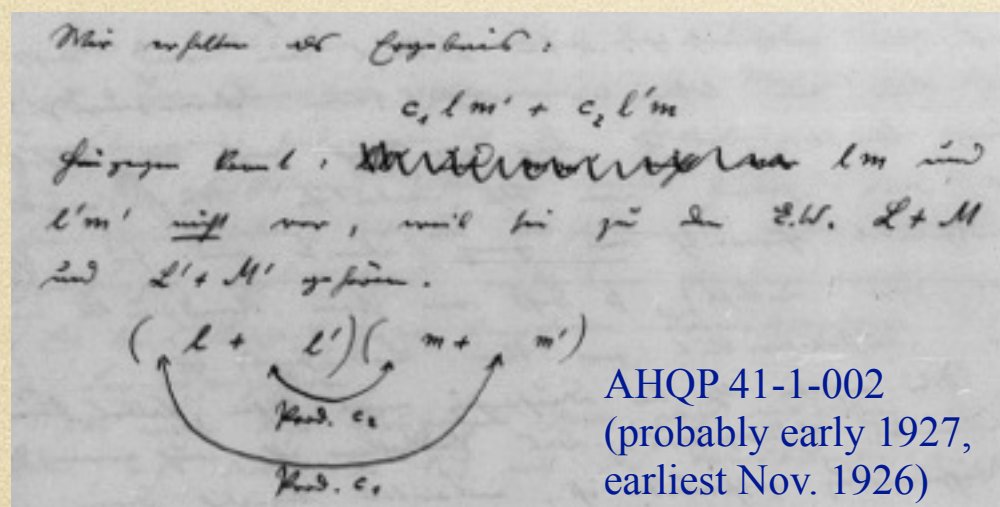
# Extension and Interpretation Many-Particle Problem

Schrödinger has one key problem with his interpretation of the wave function as a physical wave: How to make sense of its definition in **configuration space**?

In the case of  $N$  particles, what is the relation between his  $3N$ -dimensional wavefunction and a physical wave in 3 dimensions?

By mid-1926, Schrödinger attacks the **many-particle problem**, studying coupled oscillators within wave mechanics, in a hope to find a **real-space interpretation** of the many-particle wavefunction. He discusses coupled systems with Heitler and London, directly before their paper on the covalent bond (beginning of **quantum chemistry**).

In notebooks on coupled systems, Schrödinger by early 1927 has first premonition of quantum-mechanical **entanglement**.



“The combined oscillatory state, which is immediately realized upon interaction, [...] is such that it cannot be resolved anymore into the states of the component systems.”



# Conclusion

- Success of explaining “unnatural” Bose-Einstein statistics of particles as Boltzmann statistics of waves convinced Schrödinger of **wave nature of matter**.
- **First communication.** Using Hamilton’s analogy as a **heuristic** device, he derives nonrelativistic wave equation **explaining** quantum conditions of old quantum theory.
- **Second communication.** Only now, Schrödinger understood full impact of his new wave mechanics: Classical mechanics merely **limiting case** to new wave mechanics.
- Schrödinger found his own “**sharpened**” correspondence principle: the optical-mechanical analogy relates classical physics to quantum theory.
- **Classical knowledge** (Hamiltonian mechanics, Hamilton’s analogy) **crucial** for the discovery of wave mechanics.
- For Schrödinger, completed analogy crucial also for its **interpretation**: His **physical reading** of the analogy explains why attempts to reduce the new mechanics to a particle ontology must have appeared **absurd** to him.
- **Bottom line:** Even in a fundamental change of the scientific world picture, it is insufficient to describe the theoretical development as a **wholesale replacement** of one conceptual system by another. Rather, one needs to pay close attention to the intricate process of **transformation and reinterpretation** of previously accepted knowledge.