The Genesis of the New Mechanics

”A new broom sweeps clean…
…but the old broom knows the corners.“

Jürgen Renn and Christian Joas
Max Planck Institute for the History of Science, Berlin

Bari, October 2, 2009

QUANTUM HISTORY PROJECT

Outline

- **Revolution or Transformation?** The fate of the knowledge of classical physics.
- **Dizygotic twins?** The quantum revolution and the two versions of the new mechanics.
- **Classical Roots?** The refinement of the correspondence principle vs. the optical-mechanical analogy.

Part I:

Revolution or Transformation?

Challenges to the mechanical worldview

19th century physics:

- **Mechanics** (Newton, Lagrange, Hamilton)
- **Electrodynamics** (Maxwell, Hertz)
- **Thermodynamics** (Helmholtz, Clausius, Gibbs, Nernst, Boltzmann, Planck)

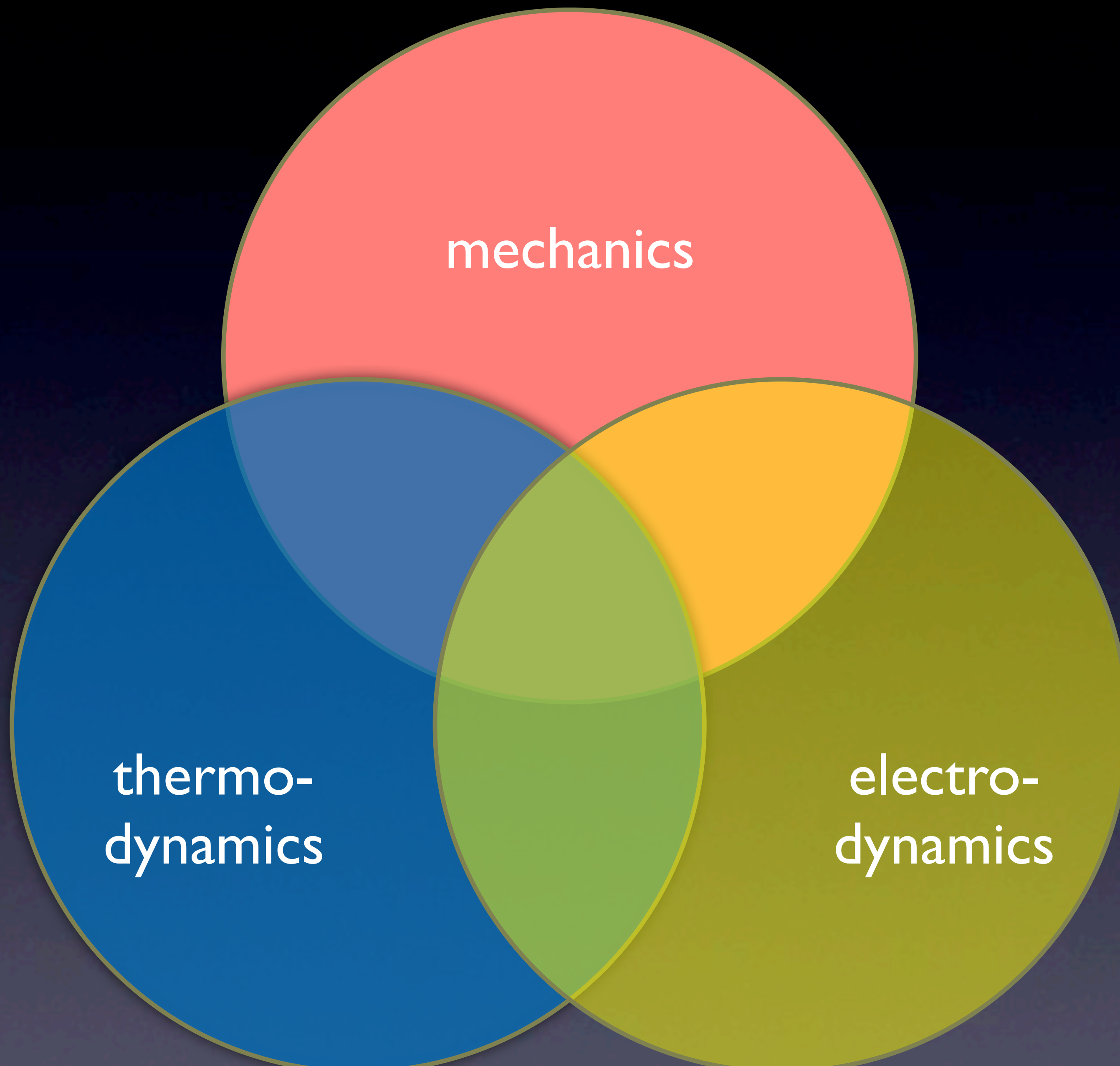
Solvay 1911

Challenges to the mechanical worldview arise at the borderline between these theories!

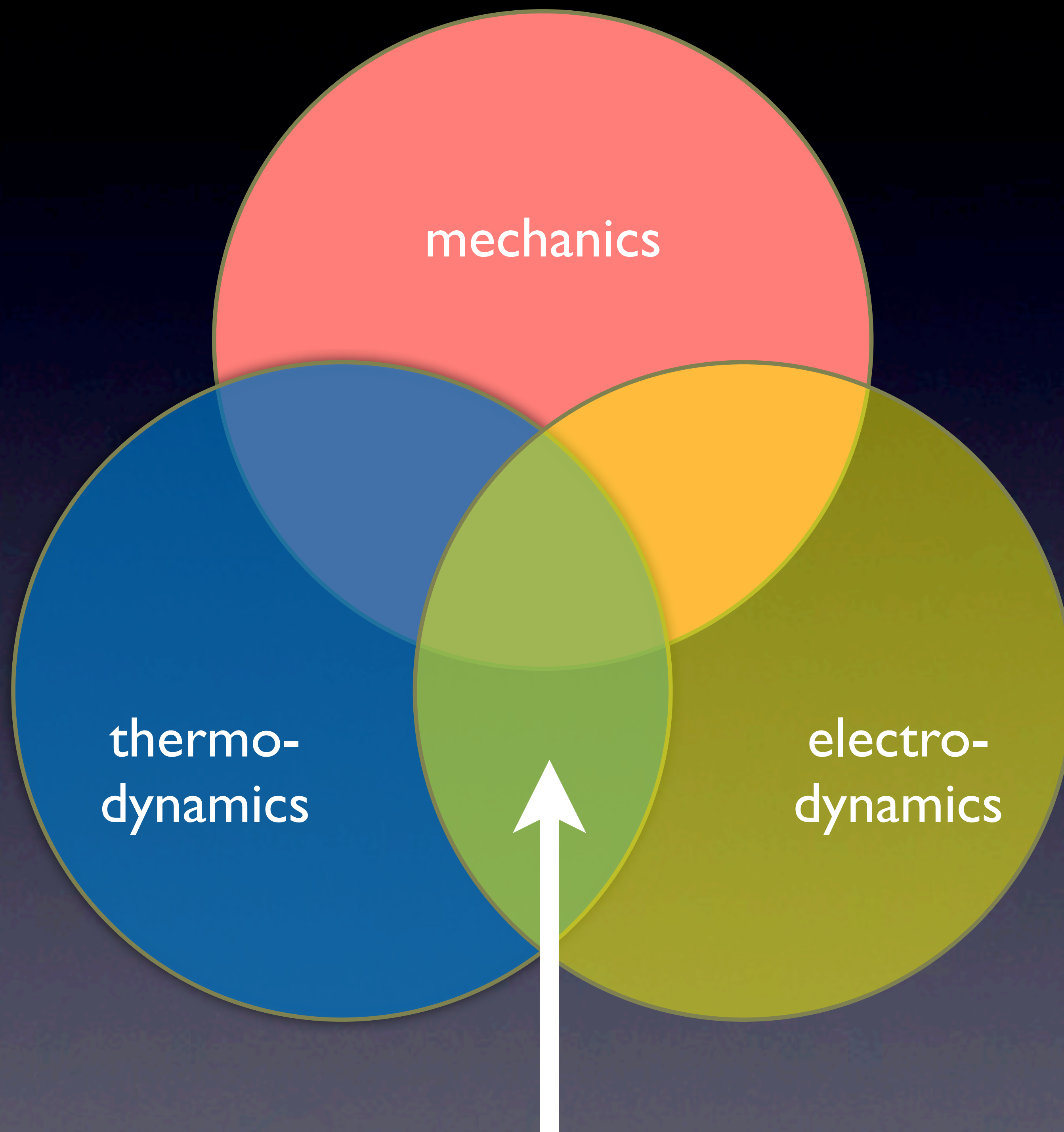
Revolution or Transformation?

- Three major **new conceptual frameworks** emerge at the beginning of the 20th century:
  - quantum physics
  - relativity physics
  - statistical physics
- Where did the **knowledge** come from that enabled the development of these frameworks?
- Which role did **previously established knowledge** play?

Borderline Problems of Classical Physics

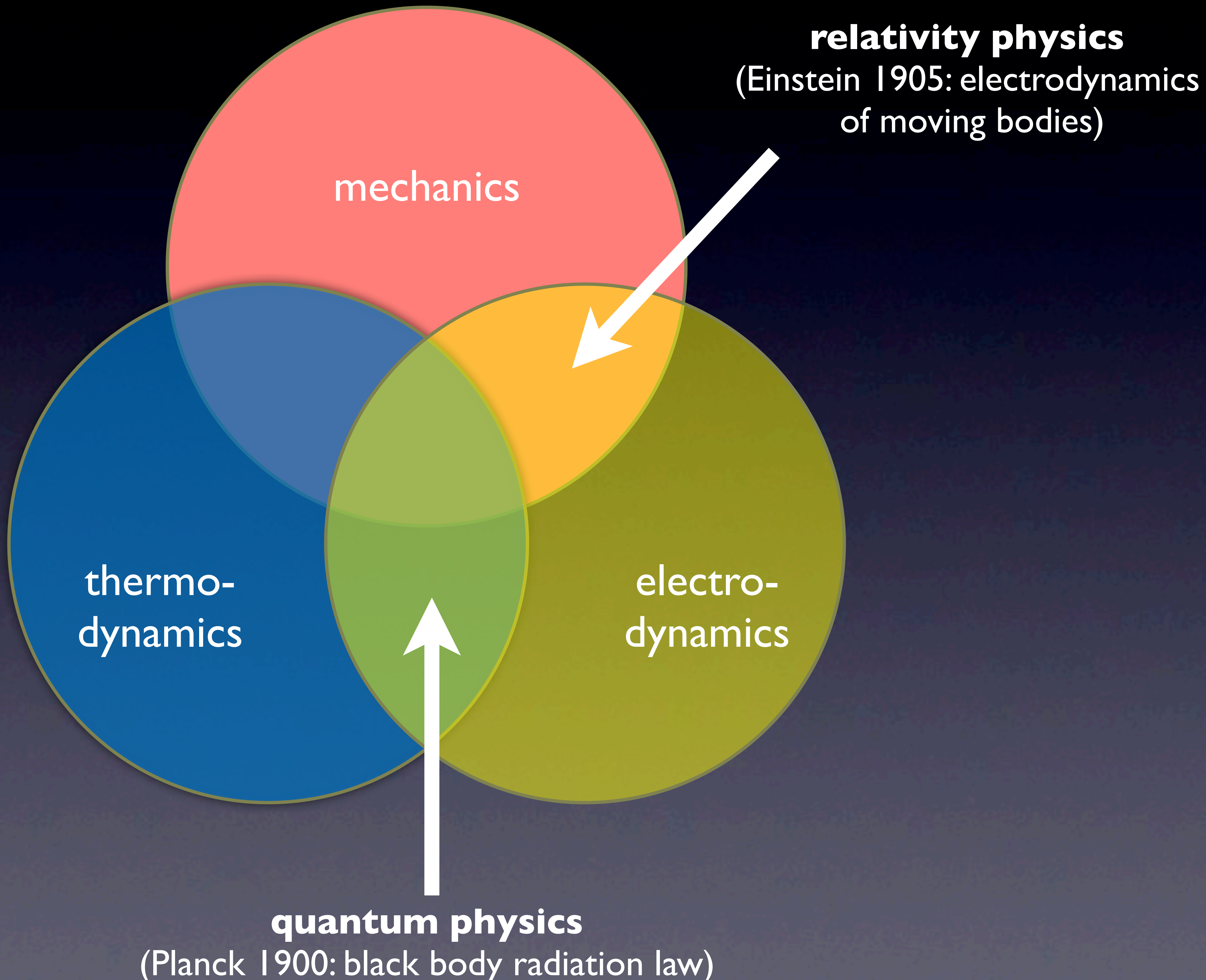


Borderline Problems of Classical Physics

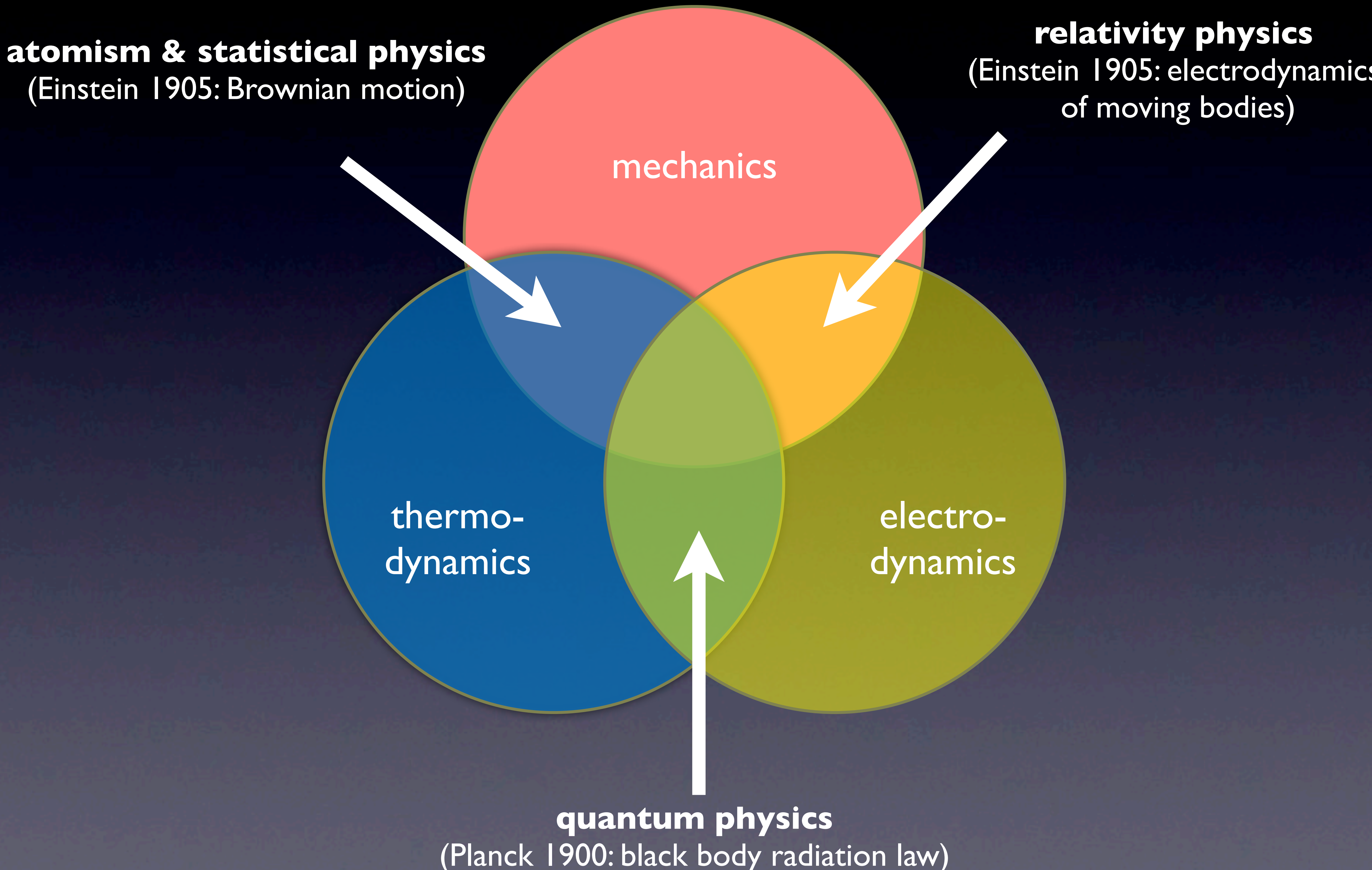


quantum physics
(Planck 1900: black body radiation law)

Borderline Problems of Classical Physics



Borderline Problems of Classical Physics

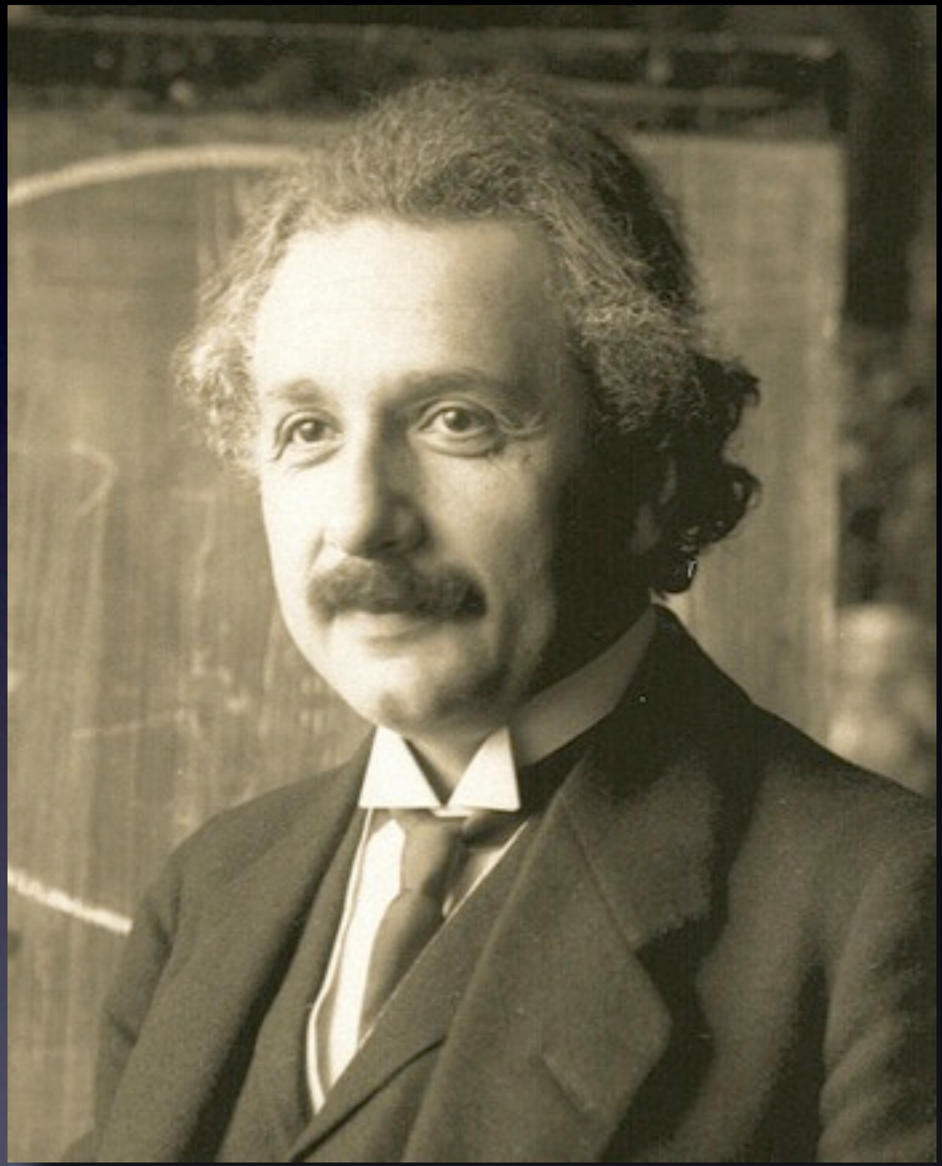


The Relativity Revolution

- The **borderline region** between mechanics and field theory includes not only the problem of light but also the problem of gravitation.
- The resolution of these problems leads to **two fundamental revisions** of the classical concepts of space and time in 1905 and 1915.
- General Relativity is the theoretical basis of modern cosmology, describing many phenomena **unknown** at the time of its creation.
- Where did the **knowledge** come from that enabled the relativity revolution?

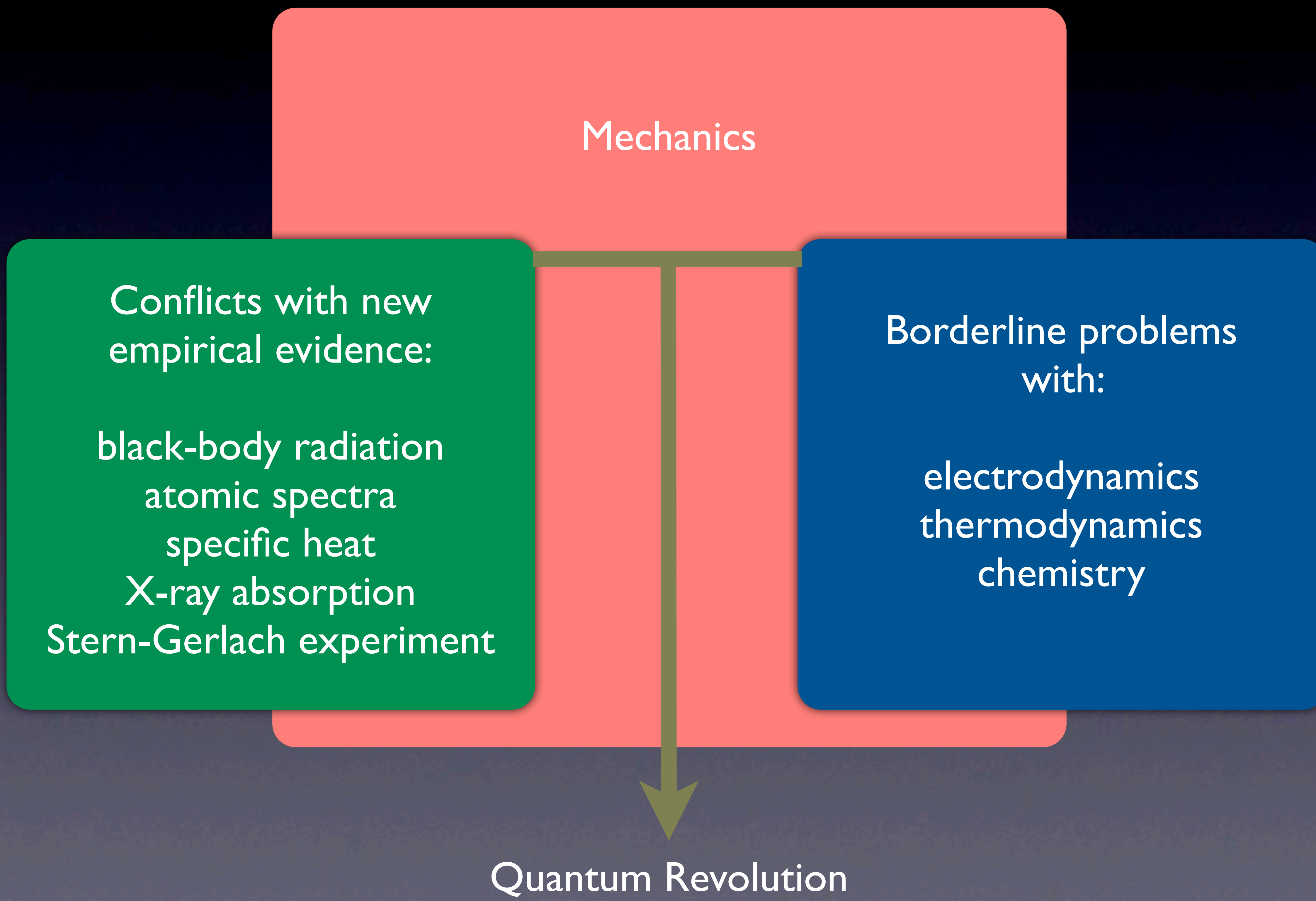
The Relativity Revolution

- The **paradox of missing knowledge**: Few empirical hints towards a theory radically different from Newton's mechanics.
- Historical research has shown: Relativity theory was the result of a **transformation of classical physics**.
- For example: Re-interpreting inertial forces as the effects of a generalized gravito-inertial field (**Equivalence Principle**).

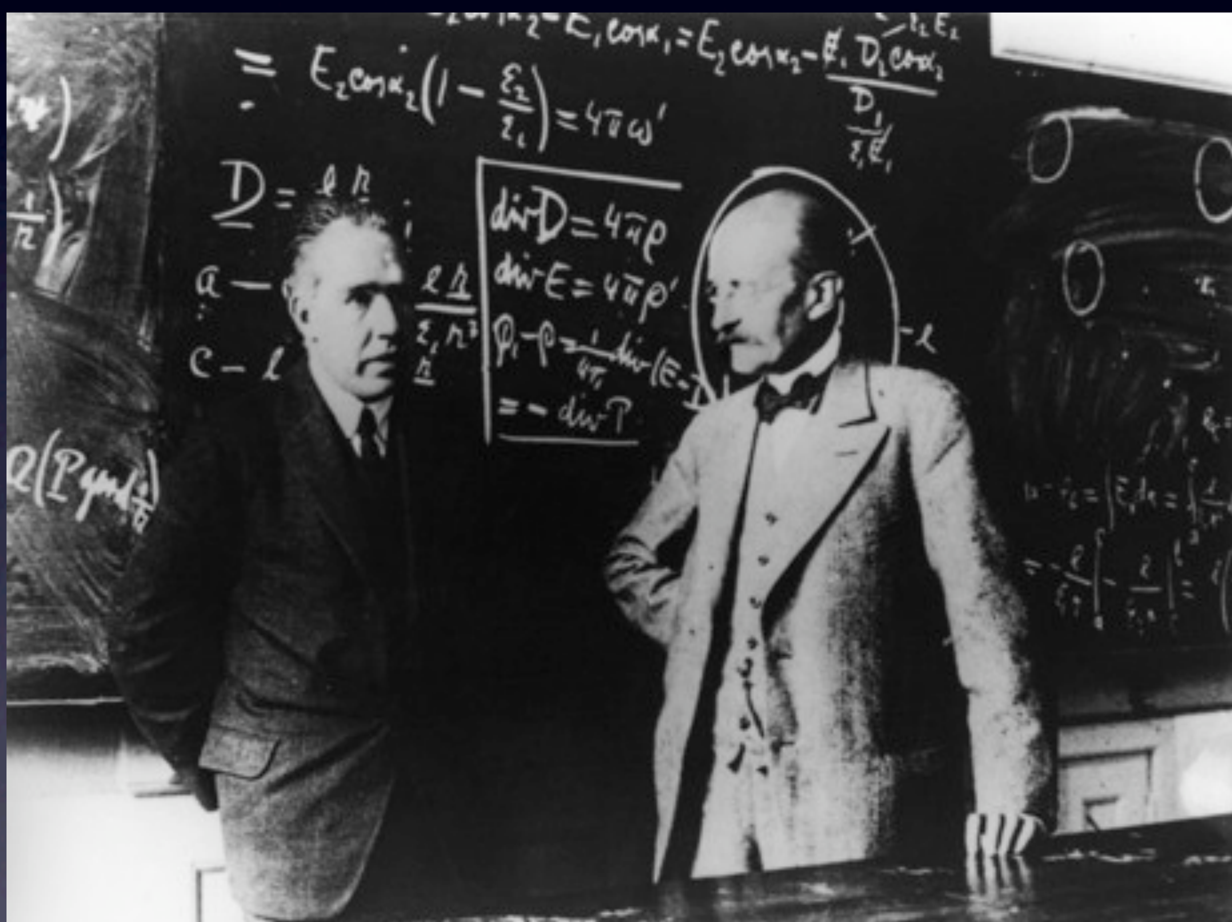


Albert Einstein (1879–1955)

The Origins of the Quantum Revolution



Historical Outline



Niels Bohr (1885–1962), Max Planck (1858–1947)

19th century: emergence of the borderline problems

1900–1911: spread of insular quantum problems

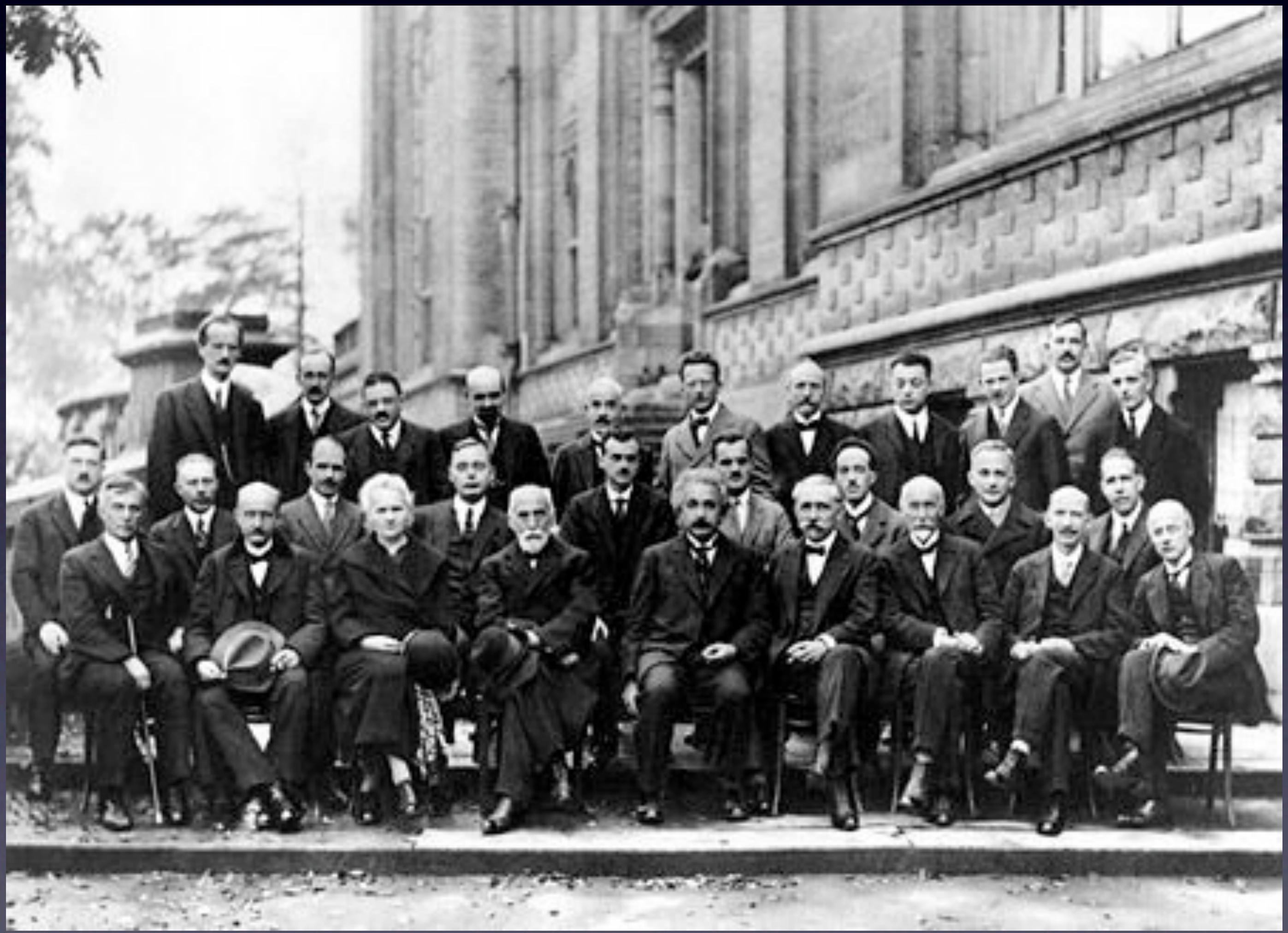
1911–1922: "old" quantum theory

1922–1925: crisis of the old quantum theory

1925–1927: emergence of matrix and wave mechanics

Quantum vs. Relativity Revolution

- Few **actors** in relativity vs. many in quantum.
- Scarce **empirical basis** in relativity vs. a bulk of new empirical findings in quantum.
- One final **formulation** in relativity vs. two distinct formulations in quantum: matrix and wave mechanics.



Solvay 1927

Old Quantum Theory

- The old quantum theory consisted in augmenting **Hamiltonian mechanics** by auxiliary conditions.
- **Quantum condition:** The action integral around a classical orbit must be an integer multiple of Planck's quantum of action:

$$\oint pdq = nh$$

- This was a **heuristic scheme** rather than full-fledged theory.
- The guiding tool in the search for quantum conditions was Bohr's **correspondence principle.**
- What were the crucial steps in the transition from old quantum theory to either matrix or wave mechanics?

The Crisis of the Old Quantum Theory

- The old quantum theory **failed** to explain many empirical findings: Helium spectrum, Zeeman effect, multiplet structure of atomic spectra, aperiodic phenomena in general.
- From ca. 1923, **doubts** in the validity of the scheme of old quantum theory arose.
- Physicists sought for an improved formulation of the **correspondence principle** that would yield refined quantum conditions with the explanatory power to tackle the open problems.
- In 1925, Heisenberg's **matrix mechanics** accomplished this feat.
- Schrödinger's 1926 **wave mechanics**, however, did not undertake a reformulation of the correspondence principle.
- Very rapidly, it became clear that the two new theories are essentially **equivalent**.
- **How can this be?**

Part II:
Dizygotic Twins?

Two New Versions of Mechanics

- Which knowledge enabled the crucial step to the two new versions of mechanics?
- How could there be two distinct approaches to what later turned out to be two versions of one and the same theory?
- Why was the reformulation of Bohr's correspondence principle crucial for one theory and immaterial for the other?

Candidates for Knowledge Fueling the Crucial Step towards Quantum Mechanics

- 1900 Planck's radiation formula for heat radiation with the help of the energy-frequency relationship
- 1905 Einstein's explanation of the photoelectric effect with the help of the light quantum hypothesis
- 1913 Bohr's explanation of the hydrogen spectrum with the help of his atomic model
- 1916 Schwarzschild's and Epstein's explanation of the Stark effect with the help of a modified Hamiltonian mechanics
- 1916 Einstein's derivation of the black-body radiation formula from the Bohr model with the help of emission and absorption coefficients
- 1923 de Broglie's explanation of Bohr's quantum conditions using a wave theory of matter
- 1924 Kramers' and Heisenberg's explanation of optical dispersion with the help of the correspondence principle
- 1924 Einstein's and Bose's explanation of Nernst's heat theorem with the help of a new statistics

Knowledge Fueling the Crucial Step towards Matrix Mechanics

- 1900 Planck's radiation formula for heat radiation with the help of the energy-frequency relationship
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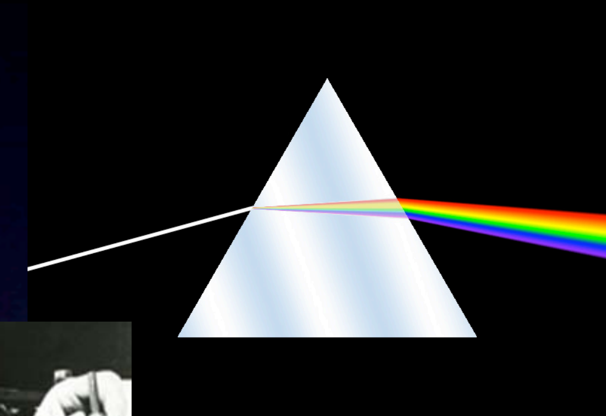
Optical Dispersion: Root of Matrix Mechanics

- **classical theories** of dispersion based on atomic models that conflicted with Bohr‘s model
- **Ladenburg 1921**: first quantum theory of dispersion
- **Kramers/BKS 1924:** Double representation of atoms:
  (a) set of Bohr orbits: unobservable
  (b) “orchestra of virtual oscillators”: carry all observable information
- **Heisenberg 1925: ”Umdeutung“** eliminates orbits entirely
- **Virtual oscillator model** played essential role in the process that led Heisenberg to quantum mechanics!



Ladenburg

$$n^2 = 1 + \frac{M_s}{\nu_s^2 - \nu^2}$$


Kramers


Heisenberg

Candidates for Knowledge Fueling the Crucial Step towards Quantum Mechanics

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Knowledge Fueling the Crucial Step towards Wave Mechanics

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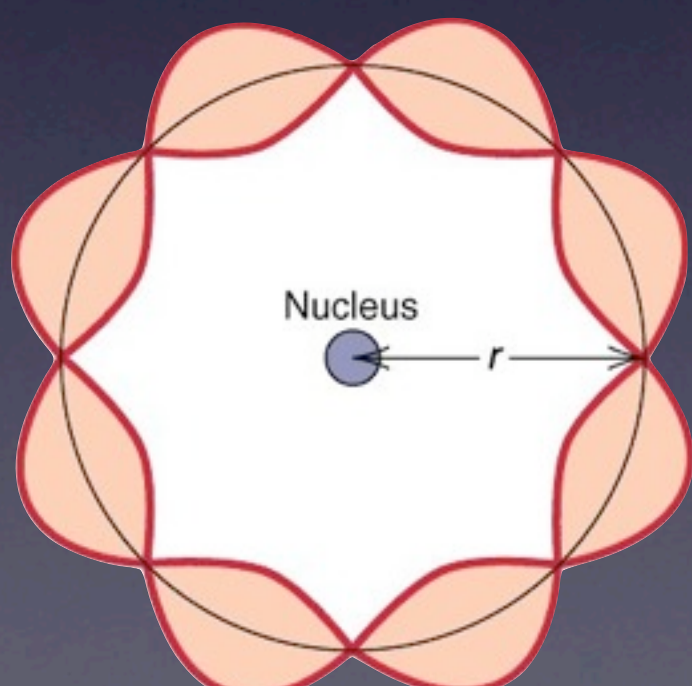
Gas Statistics and de Broglie's Matter Waves: Roots of Wave Mechanics

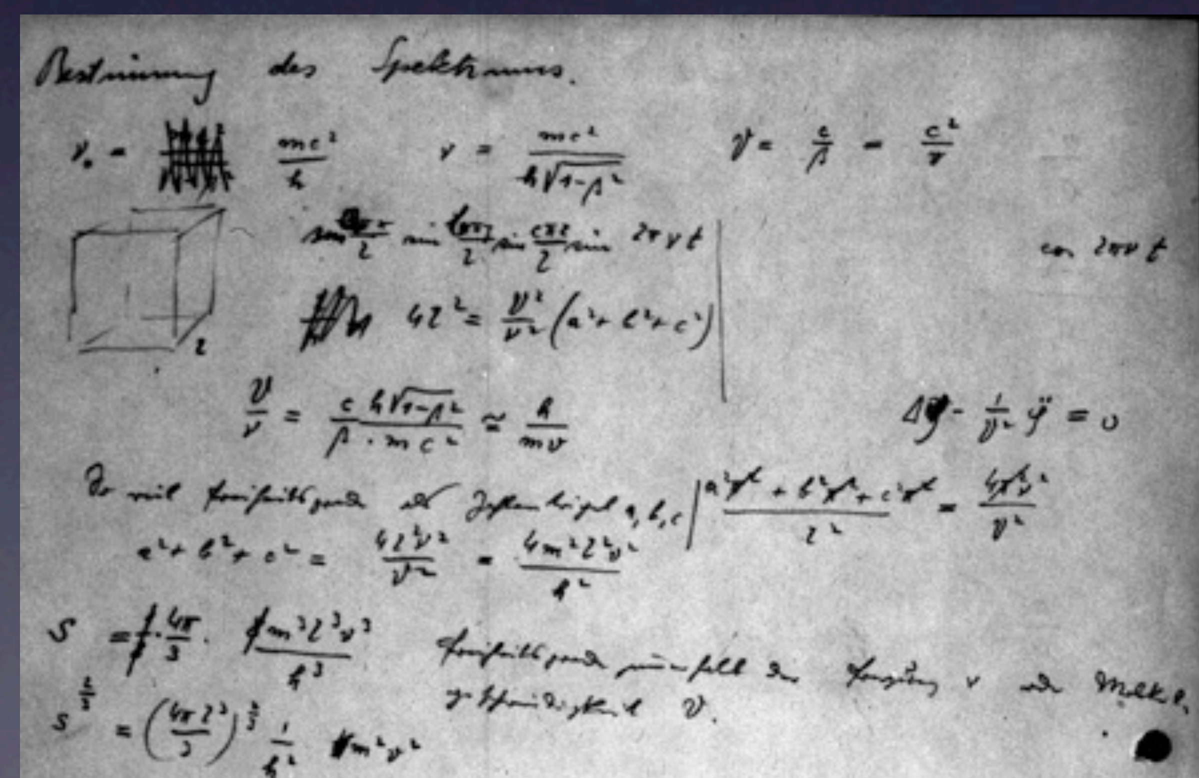
Schrödinger shows early interest in **"theoretical spectroscopy"** (1922 "On a Remarkable Property of Quantum Orbits of a Single Electron")

De Broglie's 1923 explanation of quantum orbits as a resonance phenomenon gets picked up enthusiastically by Schrödinger in 1925.



Schrödinger's central interest in 1924/25: Quantum statistics of the ideal gas.

Schrödinger tries to understand Bose-Einstein statistics and, by studying Einstein and de Broglie, discovers that it can be interpreted as **classical** Boltzmann statistics of matter waves.



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

Distinct Knowledge Resources for Matrix and Wave Mechanics?

- Crossover Phenomenon:
    - Wave mechanics grew out of attempts to explain the **hydrogen spectrum** and covered **optical dispersion** only in the aftermath.
    - Matrix mechanics grew out of attempts to explain **optical dispersion** dispersion and covered the **hydrogen spectrum** only in the aftermath.
- **How could wave mechanics come ultimately to the same conclusions as matrix mechanics without dispersion theory as an ingredient?**

Pre-established Harmony: Possible reasons?

- Was wave mechanics just a **re-dressing** of matrix mechanics which already was known to Schrödinger?
  (partly correct, because Schrödinger indeed knew matrix mechanics, but there is counter-evidence from Schrödinger's notebooks that it guided his own approach)
- Were both theories **incomplete** and did only their synthesis give rise to what we today know as quantum mechanics?
  (partly correct, because matrix mechanics provided operators and wave mechanics states, but both can be complemented with additional assumptions to explain all quantum phenomena)

Pre-established Harmony: Possible reasons?

- Does reality enforce **convergence** of different theoretical approaches?
  (partly correct, because both theories are connected to contemporary empirical evidence, but both theories cover only aspects of the quantum reality, and those aspects happen to be essentially the same ones. They failed to cover other aspects also playing a role at the time, like spin, relativity, statistics.)

- Were pre-existing **mathematical structures**, such as the Hilbert space formalism, only uncovered by the two approaches?
  (partly correct, because the equivalence of the two approaches was indeed soon recognized by Schrödinger and others, but there is no historical evidence that the mathematical relation between the two theories played a heuristic role guaranteeing the harmony of both approaches in advance.)

Pre-established Harmony: **the genetic view**

- Both are transformations of a **common ancestor**: old quantum theory!
- Rationale: Find a **modification of the scheme of old quantum theory** integrating the new knowledge about the interaction between matter and elelctromagnetic fields as part of the formalism rather than as an auxiliary condition, like in the old quantum theory.
- The key element of the new knowledge was Ritz's combination principle and the **energy-frequency condition**.

Heisenberg 1925: Matrix Mechanics

- Heisenberg re-cast the correspondence principle through his "Umdeutung" of mechanical quantities.
- The sharpened correspondence led Heisenberg from Hamiltonian mechanics to his new matrix mechanics.


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.

Heisenberg

Hamiltonian Mechanics → Correspondence Principle → Matrix Mechanics

Schrödinger 1926: Wave Mechanics


Quantisierung als Eigenwertproblem
(Erste Mitteilung)
(Annalen der Physik (4) Bd. 79, 1926)

§ 1. In dieser Mitteilung möchte ich zunächst an dem ein-
fachsten Fall des (nichtrelativistis
stoffatoms zeigen, daß die üblich
durch eine andere Forderung ers
von „ganzen Zahlen" mehr vork
die Ganzzahligkeit auf dieselbe
Ganzzahligkeit der *Knotenzahl* ei
neue Auffassung ist verallgemeine
glaube, sehr tief an das wahre W
Die übliche Form der letzt
tonsche partielle Differentialgleic

(1) $H\left(q, \frac{\partial S}{\partial q}\right)$

Es wird von dieser Gleichung
sich darstellt als *Summe* von Fun
unabhängigen Variablen q.
Wir führen nun für S eine
daß ψ als ein *Produkt* von eingriffi
Koordinaten erscheinen würde.

(2) $S = K \lg$

Die Konstante K muß aus dimen
werden, sie hat die Dimension einer

(1') $H\left(q, \frac{K}{\psi} \frac{\partial}{\partial}\right.$

Wir suchen nun *nicht* eine Lösun
wir stellen folgende Forderung.
Vernachlässigung der Massenverän
sichtigung derselben wenigstens da
elektronenproblem handelt, auf die

— 82 —

Schrödinger

- Schrödinger found a „wave" generalization of Hamiltonian mechanics through the optical-mechanical analogy.
- This led him to his new mechanics.
- This also explains Schrödinger's later stance on interpretation.

Hamiltonian Mechanics → Optical-Mechanical Analogy → Wave Mechanics

Part III:
Classical Roots

Heisenberg's Re-Casting of the Correspondence Principle

Die Antwort lautet klassisch offenbar so:

$$\mathfrak{B}_\beta(n)\, e^{i\,\omega(n)\,\beta t} = \sum_{-\infty}^{+\infty}{}_{\alpha}\, \mathfrak{A}_\alpha\, \mathfrak{A}_{\beta-\alpha}\, e^{i\,\omega(n)\,(\alpha+\beta-\alpha)\,t} \quad (3)$$

bzw.

$$= \int_{-\infty}^{+\infty} \mathfrak{A}_\alpha\, \mathfrak{A}_{\beta-\alpha}\, e^{i\,\omega(n)\,(\alpha+\beta-\alpha)\,t}\, d\alpha, \quad (4)$$

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

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

bzw.

$$= \int_{-\infty}^{+\infty} d\alpha\, \mathfrak{A}(n, n-\alpha)\, \mathfrak{A}(n-\alpha, n-\beta)\, e^{i\,\omega(n,n-\beta)\,t}; \quad (8)$$

und zwar ergibt sich diese Art der Zusammensetzung nahezu zwangläufig aus der Kombinationsrelation der Frequenzen. Macht man diese An-

Heisenberg‘s Re-Casting of the Correspondence Principle

$$\oint m\dot{x}^2\,dt = 2\pi m \sum_{-\infty}^{+\infty}{}^{\alpha} \left| a_\alpha(n) \right|^2 \alpha^2 \omega_n. \tag{14}$$

Dieses Phasenintegral hat man bisher meist gleich einem ganzen Vielfachen von h, also gleich $n \,.\, h$ gesetzt; eine solche Bedingung fügt sich aber nicht nur sehr gezwungen der mechanischen Rechnung ein, sie erscheint auch selbst vom bisherigen Standpunkt aus im Sinne des Korrespondenzprinzips willkürlich; denn korrespondenzmäßig sind die J nur bis auf eine additive Konstante als ganzzahlige Vielfache von h festgelegt, und an Stelle von (14) hätte naturgemäß zu treten:

$$\frac{d}{dn}(nh) = \frac{d}{dn} \cdot \oint m\dot{x}^2\,dt,$$

das heißt

$$h = 2\pi m \cdot \sum_{-\infty}^{+\infty}{}^{\alpha} \alpha \frac{d}{dn}\left(\alpha\omega_n \cdot \left| a_\alpha \right|^2\right). \tag{15}$$

Heisenberg‘s Re-Casting of the Correspondence Principle

Zwar besitzt eben nur Gleichung (15) eine an die Kramerssche Dispersionstheorie anknüpfende einfache quantentheoretische Verwandlung [1]):

$$h = 4\pi m \sum_0^\infty \alpha \left\{ |a(n, n+\alpha)|^2 \omega(n, n+\alpha) - |a(n, n-\alpha)|^2 \omega(n, n-\alpha) \right\}, \quad (16)$$

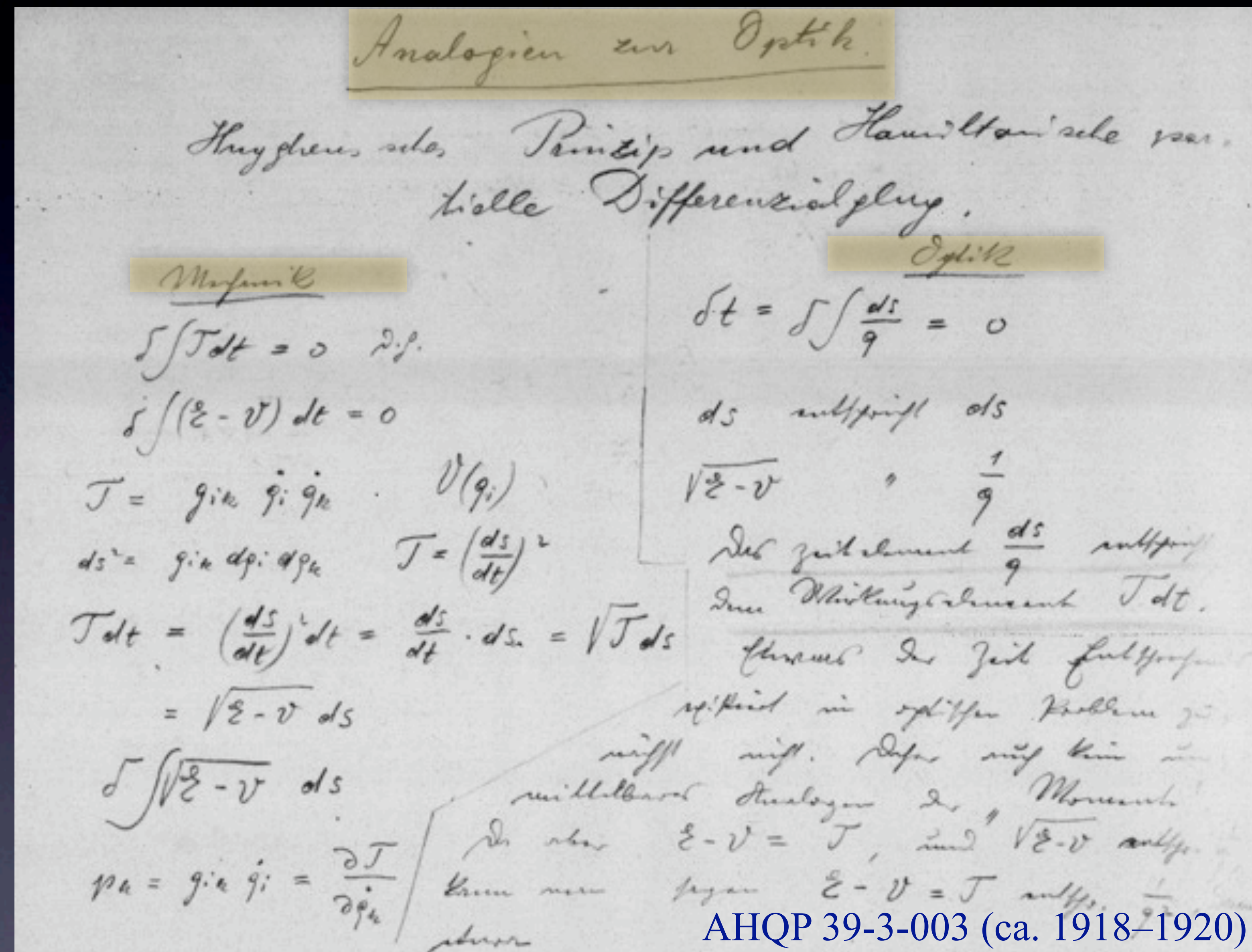
doch diese Beziehung genügt hier zur eindeutigen Bestimmung der a; denn die in den Größen a zunächst unbestimmte Konstante wird von selbst durch die Bedingung festgelegt, daß es einen Normalzustand geben solle, von dem aus keine Strahlung mehr stattfindet; sei der Normalzustand mit n_0 bezeichnet, so sollen also alle

$$a(n_0, n_0 - \alpha) = 0 \quad (\text{für } \alpha > 0)$$

sein. Die Frage nach halbzahliger oder ganzzahliger Quantelung dürfte daher in einer quantentheoretischen Mechanik, die nur Beziehungen zwischen beobachtbaren Größen benutzt, nicht auftreten können.

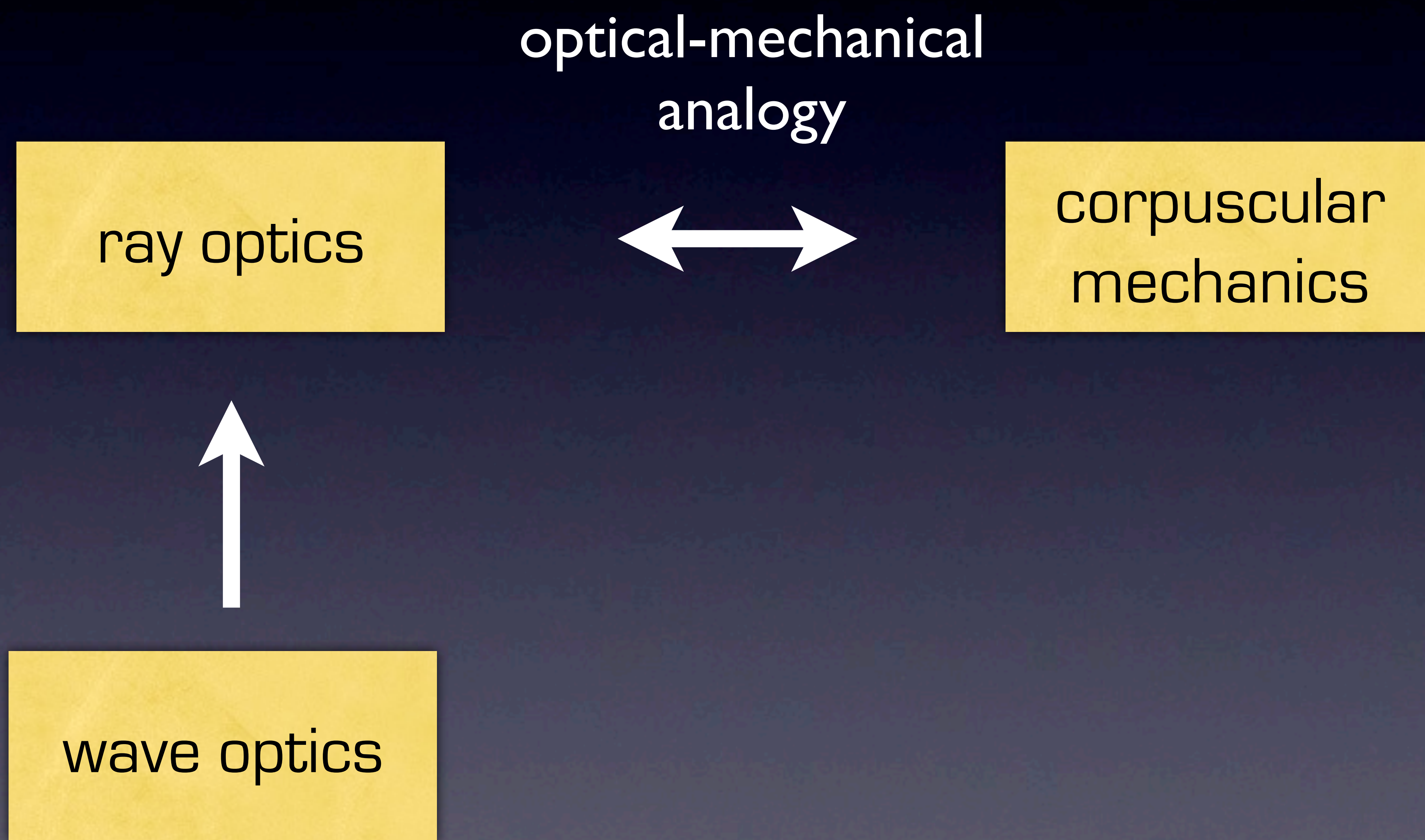
Schrödinger's Completion of Hamilton's Analogy

- Schrödinger did not worry about the absence of mechanical frequencies in quantum phenomena, but sought a way to derive quantum conditions from within mechanics, **already as early as 1918**.
- Early notebooks show attempts at explaining **quantum conditions** as **constraints** in a generalized Hertzian mechanics.
- In this context, he encounters **Hamilton's optical-mechanical analogy** from 1834.



Schrödinger's notebook (ca. 1918–1920) on Tensor-Analytic Mechanics: Hamilton's analogy between mechanics (left) and optics (right).

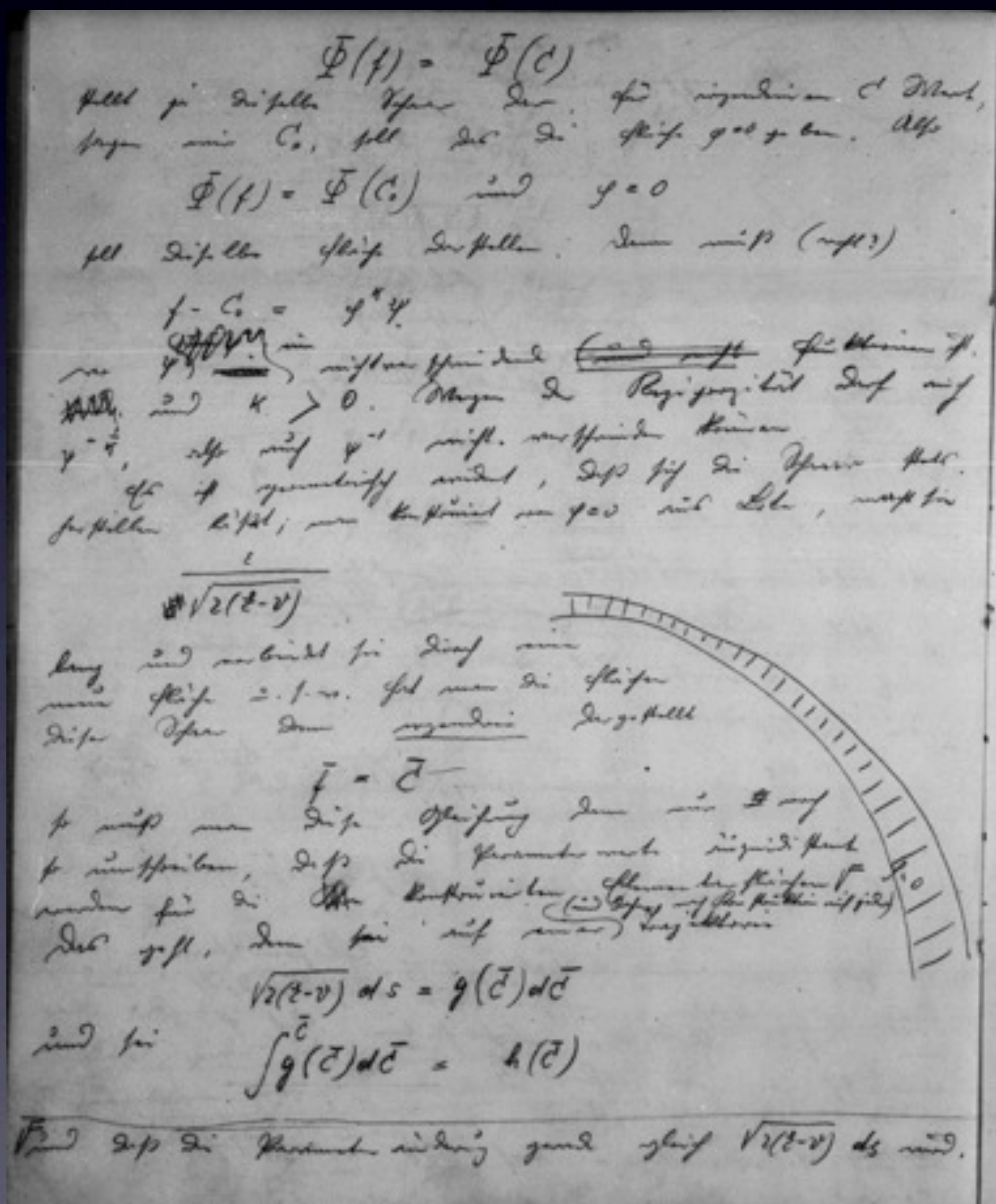
Schrödinger's Completion of Hamilton's Analogy: The Optical-Mechanical Analogy



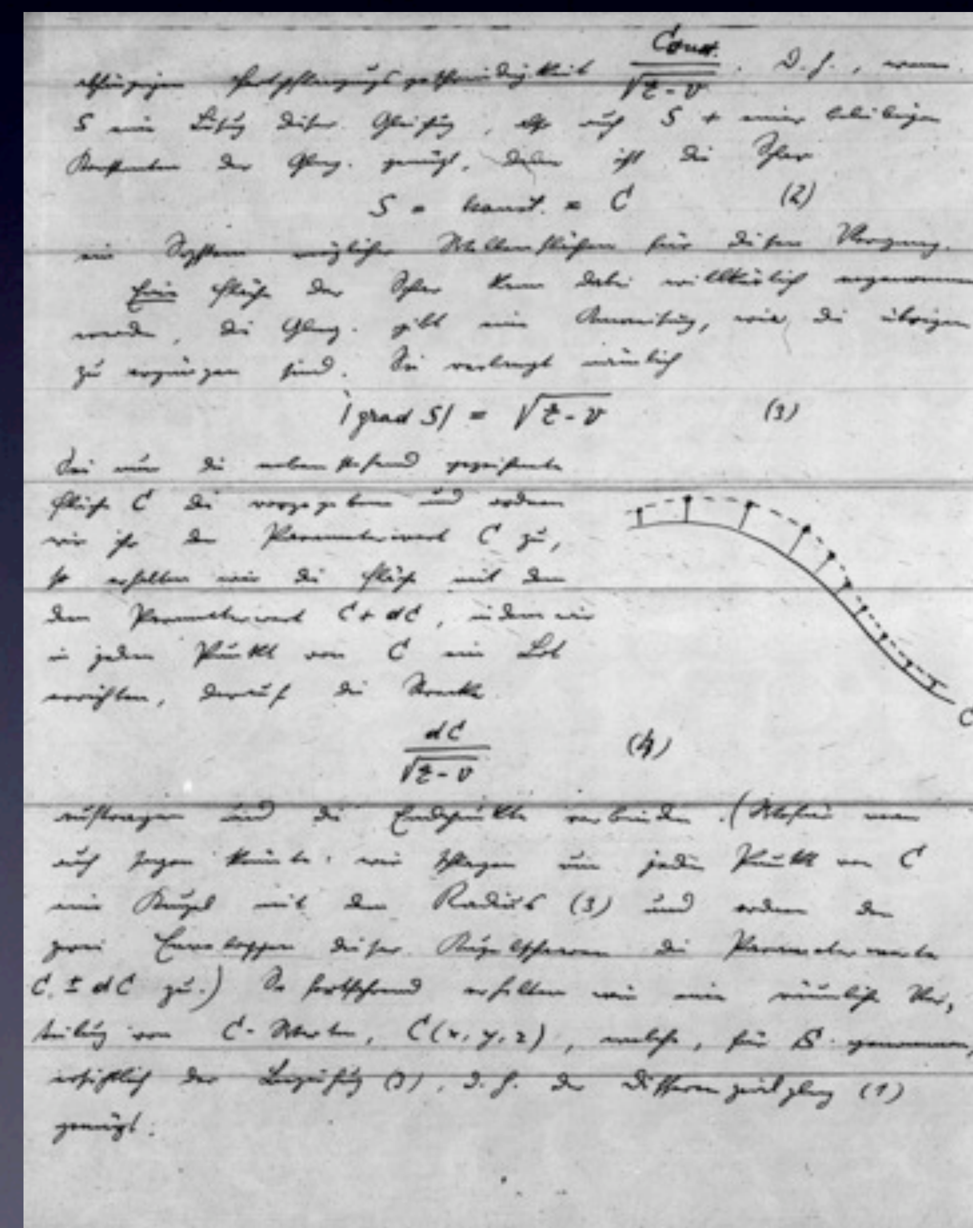
abstract attempt at unifying optics and mechanics

Schrödinger's Completion of Hamilton's Analogy

Reappearance of the analogy in 1925-1926 notebooks

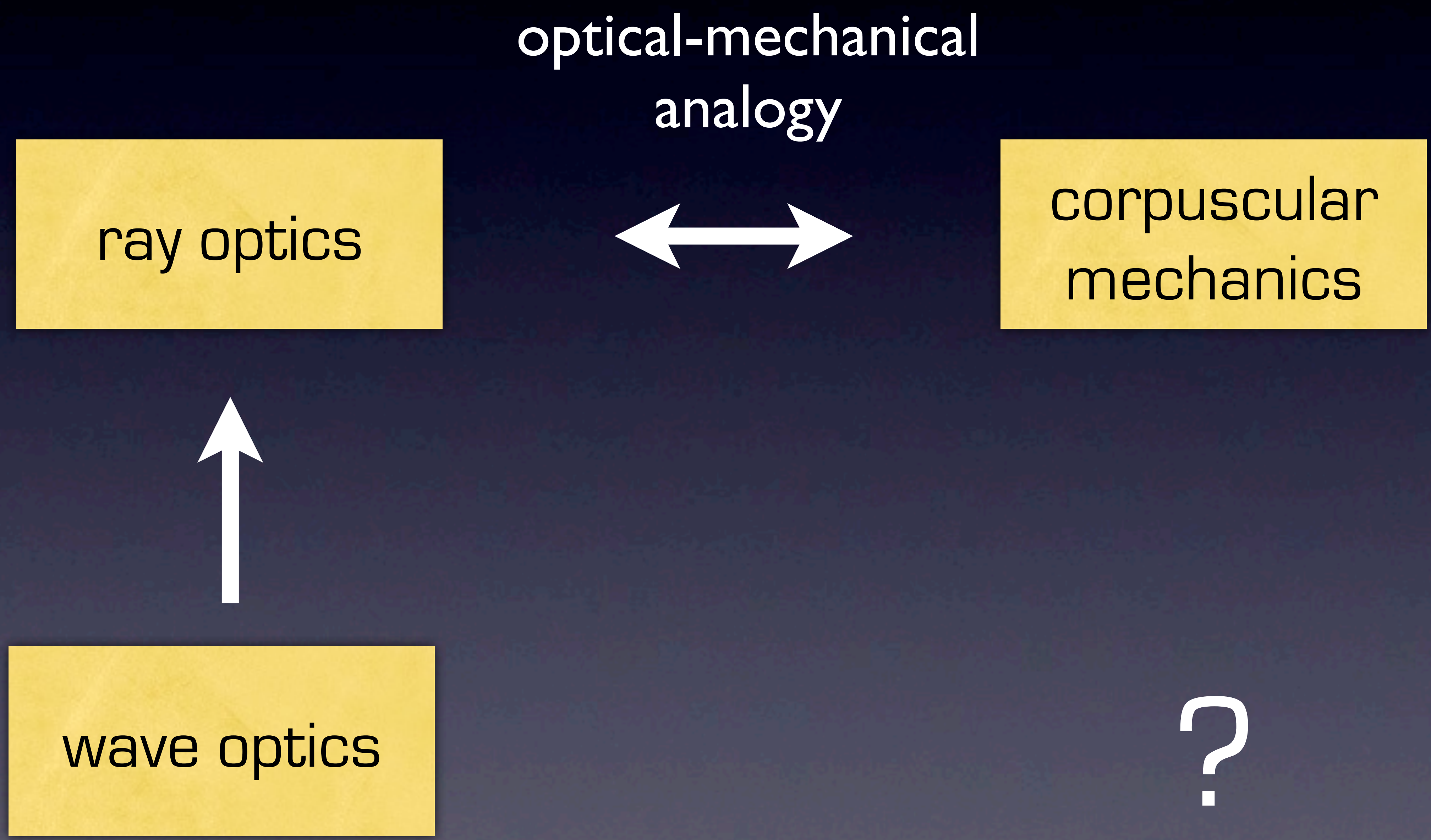


Notebook "Tensor-Analytic Mechanics"
AHQP 39-3-001 (ca. 1918–1920)

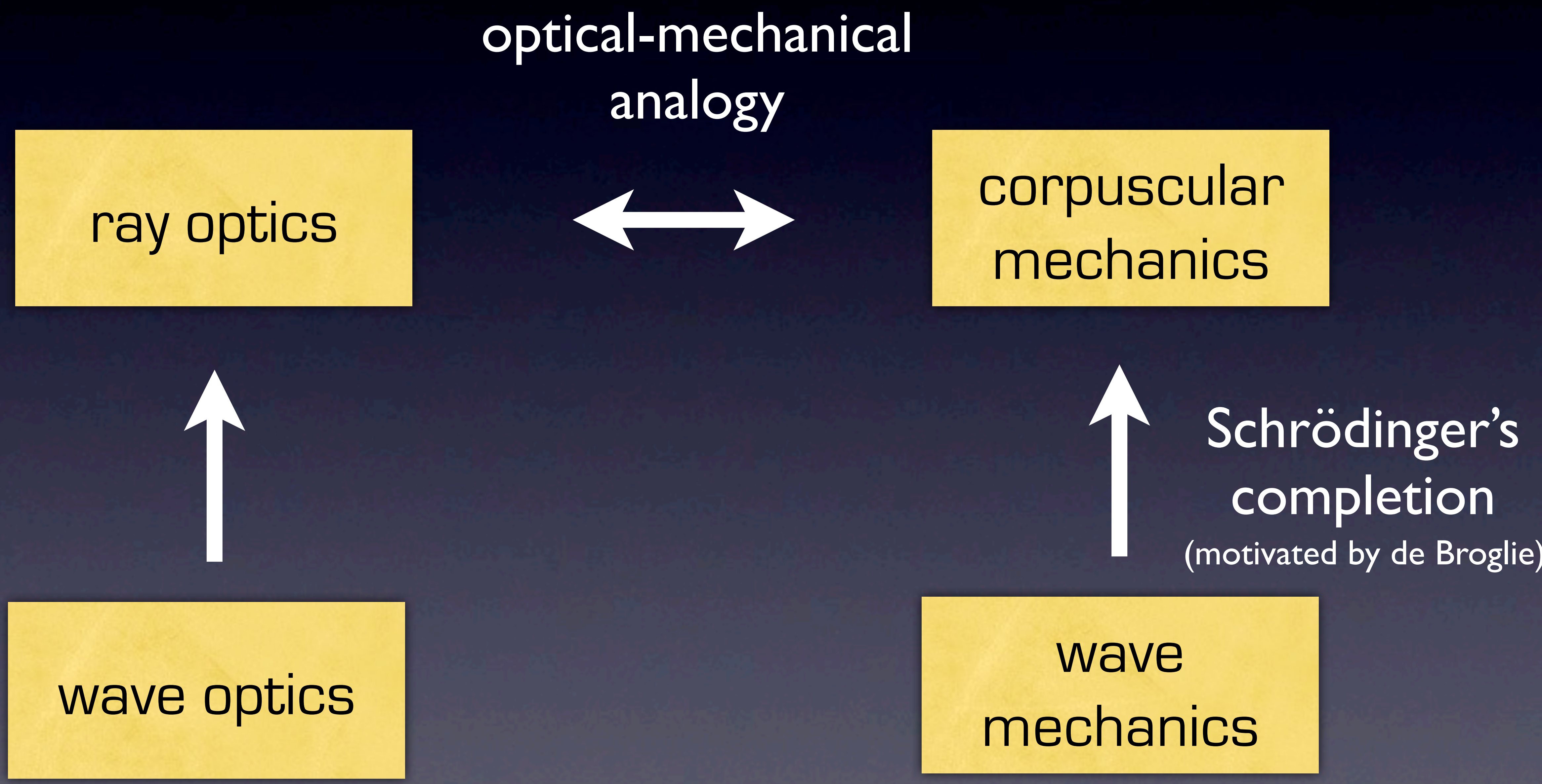


Notebook "Eigenvalue Problem of the Atom II."
AHQP 40-6-001 (ca. Feb. 1926)

Schrödinger's Completion of Hamilton's Analogy



Schrödinger's Completion of Hamilton's Analogy



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

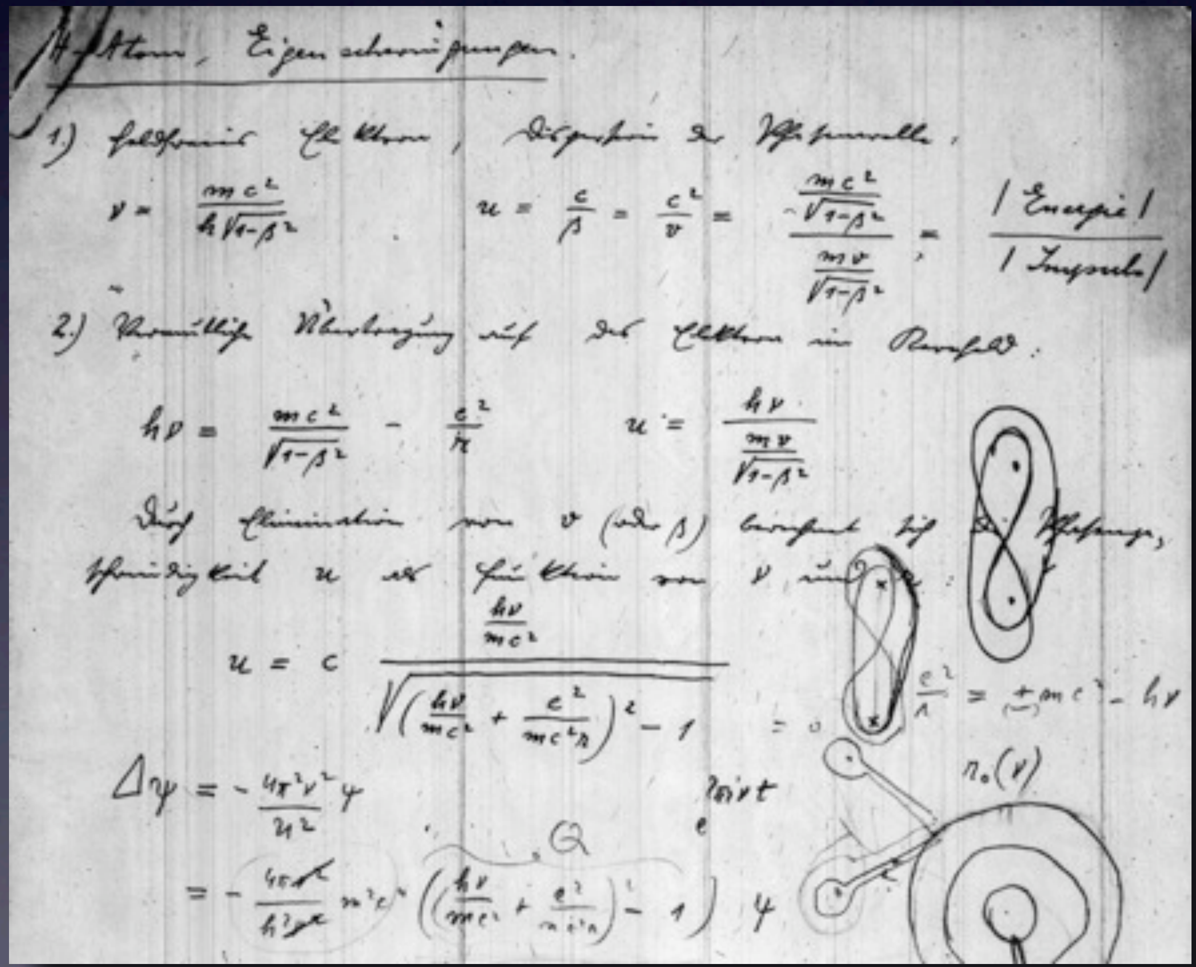
Schrödinger's Completion of Hamilton's Analogy

- Schrödinger encounters the analogy again in de Broglie in late 1925 and completes the analogy: The new mechanics is more general than Hamiltonian mechanics in the same sense as wave optics is more general than ray optics!

- Schrödinger did not re-cast the correspondence principle but he re-cast the old mechanics instead.

- The optical-mechanical analogy offers a heuristically attractive justification for the introduction of a wave function and the search for a wave equation: **the quantization rules of old quantum theory can be explained as eigenvalue problems of a partial differential equation**

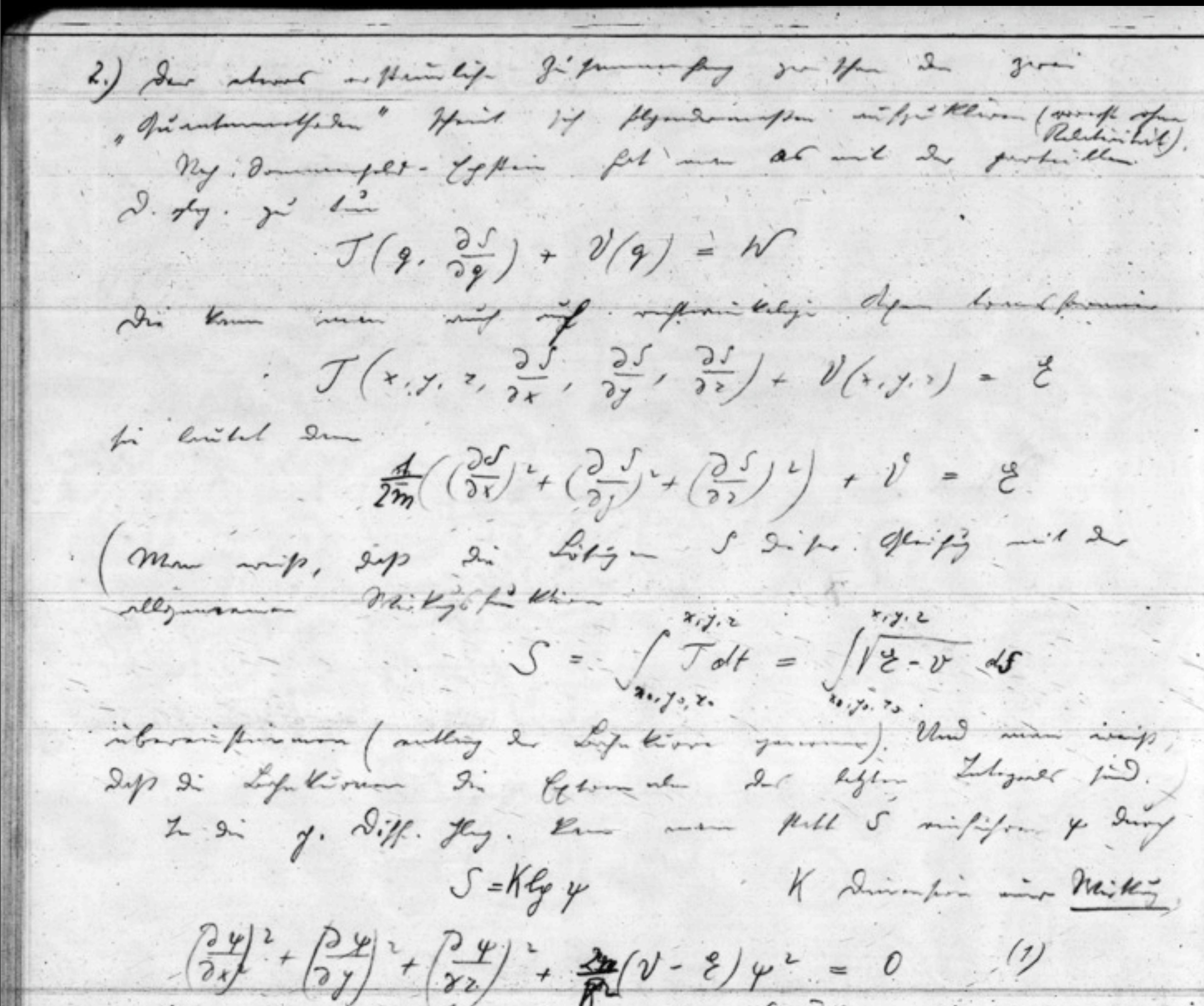
- Through the optical-mechanical analogy, he gets the correspondence principle „for free".



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

Schrödinger's Completion of Hamilton's Analogy

Confrontation with the old quantum theory:



„der etwas erstaunliche Zusammenhang zwischen den zwei ‚Quantenmethoden'"

„the somewhat astonishing relation between the two ‚quantum methods'"

The Genesis of the New Mechanics

- Both matrix and wave mechanics share a **common ancestor**: old quantum theory!
- Old quantum theory is both
    - a **set of ingenious solutions** to insular quantum problems
    - an approach to unite **Hamiltonian mechanics** with the energy-frequency relation
- **What can we learn from this "genetics" of quantum mechanics?**

The Genesis of the New Mechanics

- Early quantum mechanics deals with a **coupling of mechanics and electro-magnetic fields** and refers to the new empirical knowledge at the interface between matter and radiation.
- In classical physics, the **Lorentz force** was responsible for the coupling of nonrelativistic mechanics and intrinsically relativistic electrodynamics.
- **But this bridge has collapsed:** Optical dispersion can neither be described by an elastically bound electron, nor by atoms on Bohr orbits. The frequencies come out wrong.
- In early quantum mechanics, the **Schrödinger equation** takes the place of the Lorentz force in classical physics. Like the Lorentz force, the Schrödinger equation describes the effect of the electromagnetic field on matter.
- Heitler-London (1927) recognize this and build a new „quantum“ chemistry on this insight.

[1] Es ist nicht überflüssig, darauf hinzuweisen, daß der hierin angenommene Zusammenhang zwischen wellenmechanischer Frequenz und mechanischer Energie durchaus hypothetisch ist, denn wir wissen, daß gerade der Lorentzsche Kraftansatz, der die Einwirkung des Feldes auf die Materie beherrscht, in der Quantenmechanik durch etwas ganz anderes, nämlich die Wellengleichung ersetzt wird.

Heitler-London (1927)

Conclusion

- The two new versions of mechanics both constitute a **transformation** of Hamiltonian mechanics in the light of the energy-frequency relation.
- Heisenberg re-casts the **correspondence principle** in order to conserve the formal structure of Hamiltonian mechanics.
- Schrödinger completes **Hamilton's optical-mechanical analogy** and generalizes Hamiltonian mechanics.
- The role of the optical-mechanical analogy is reminiscent of the role the **equivalence principle** played for Einstein in his derivation of general relativity. Just as Einstein did when elaborating the consequences of the equivalence principle, Schrödinger realized an **unused potential of classical physics** when completing Hamilton's analogy.

QUANTUM HISTORY PROJECT

Schrödinger's Completion of Hamilton's Analogy

Confrontation with the old quantum theory: