Pathways from Classical to Quantum Physics

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QUANTUM HISTORY PROJECT

Outline

- **Revolution or Transformation?** The fate of the knowledge of classical physics.
- **Fraternal 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)

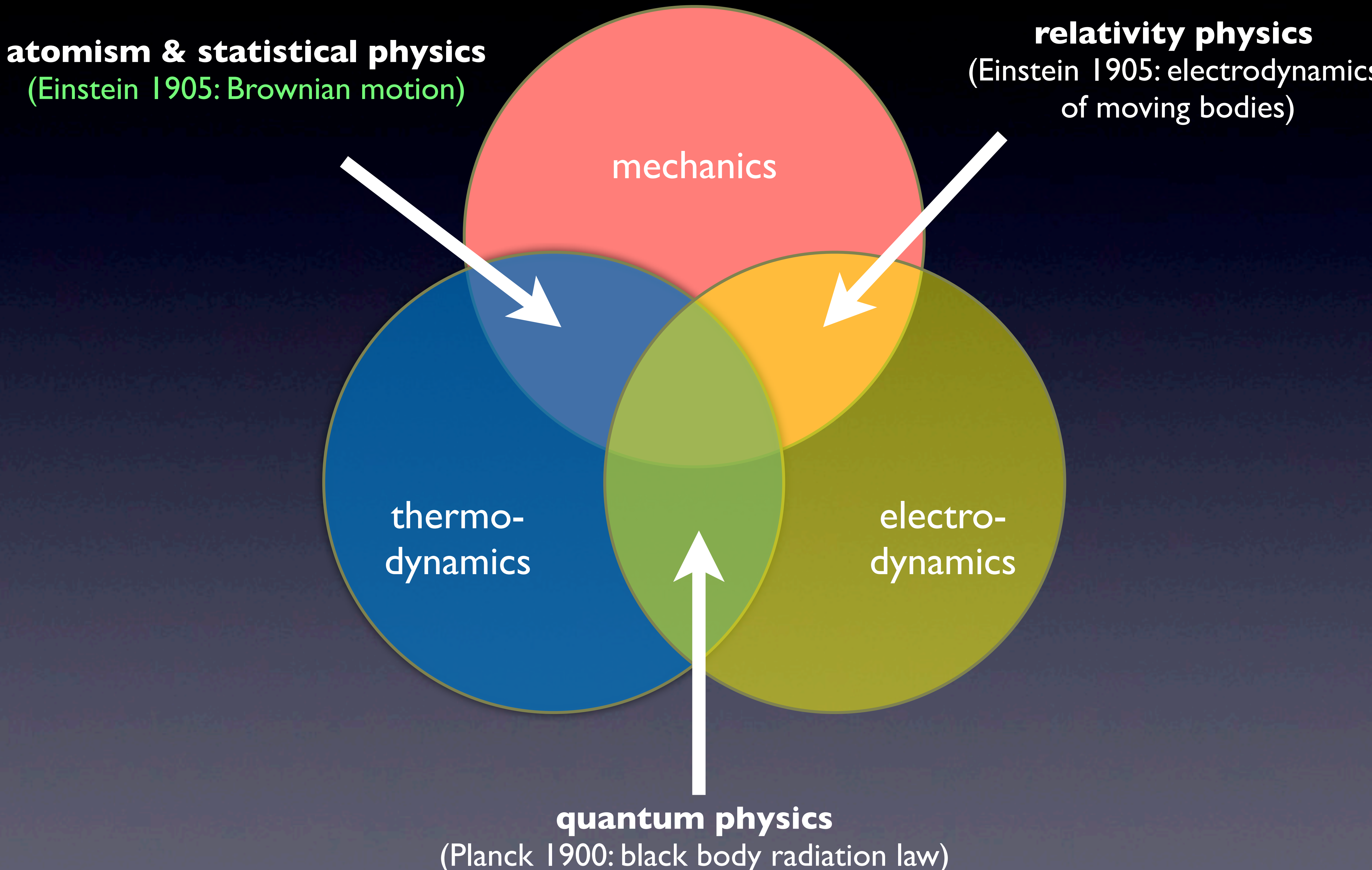
Solvay 1911

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

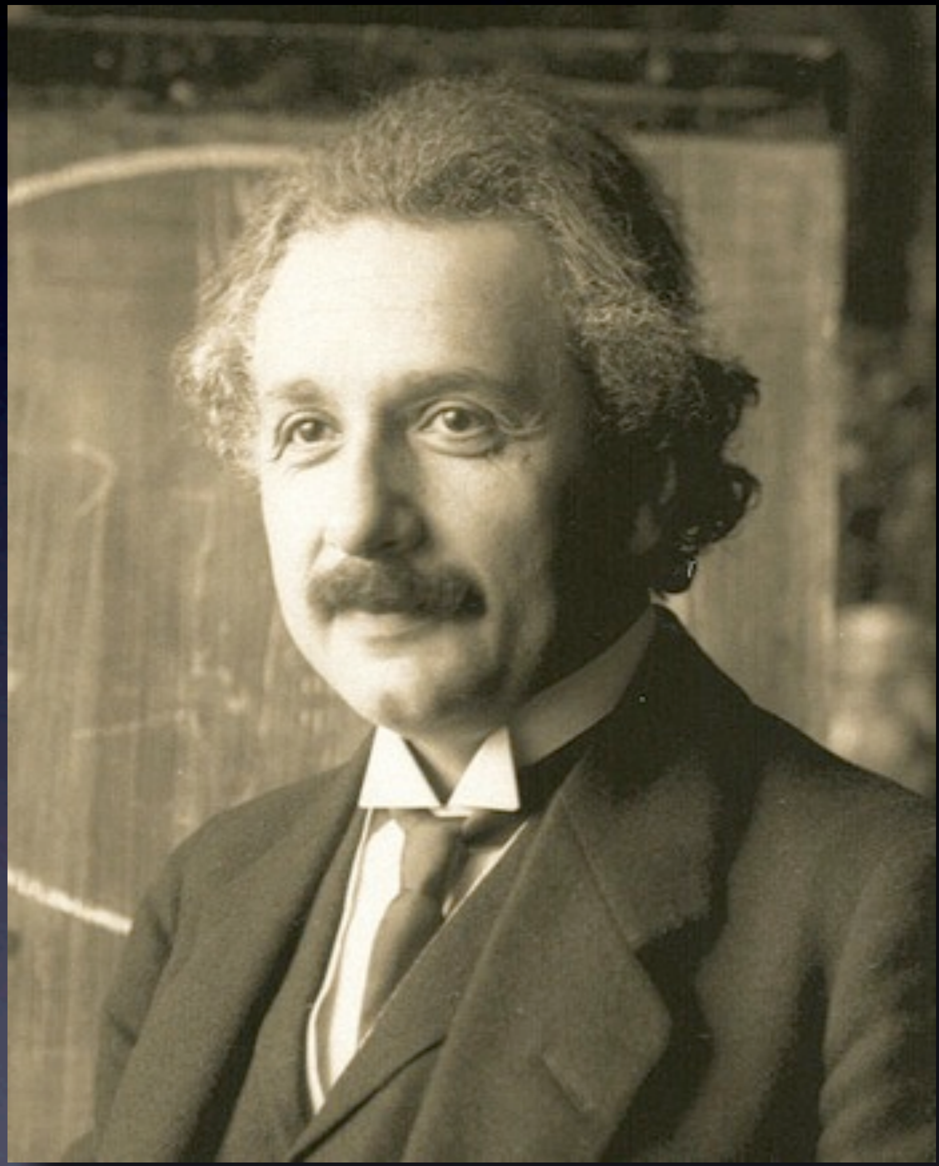


The Relativity Revolution

- 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 a **transformation of classical physics** resulting from a **reorganization** of established knowledge under new principles.
- For example: Re-interpreting inertial forces as the effects of a generalized gravito-inertial field (**Equivalence Principle**).

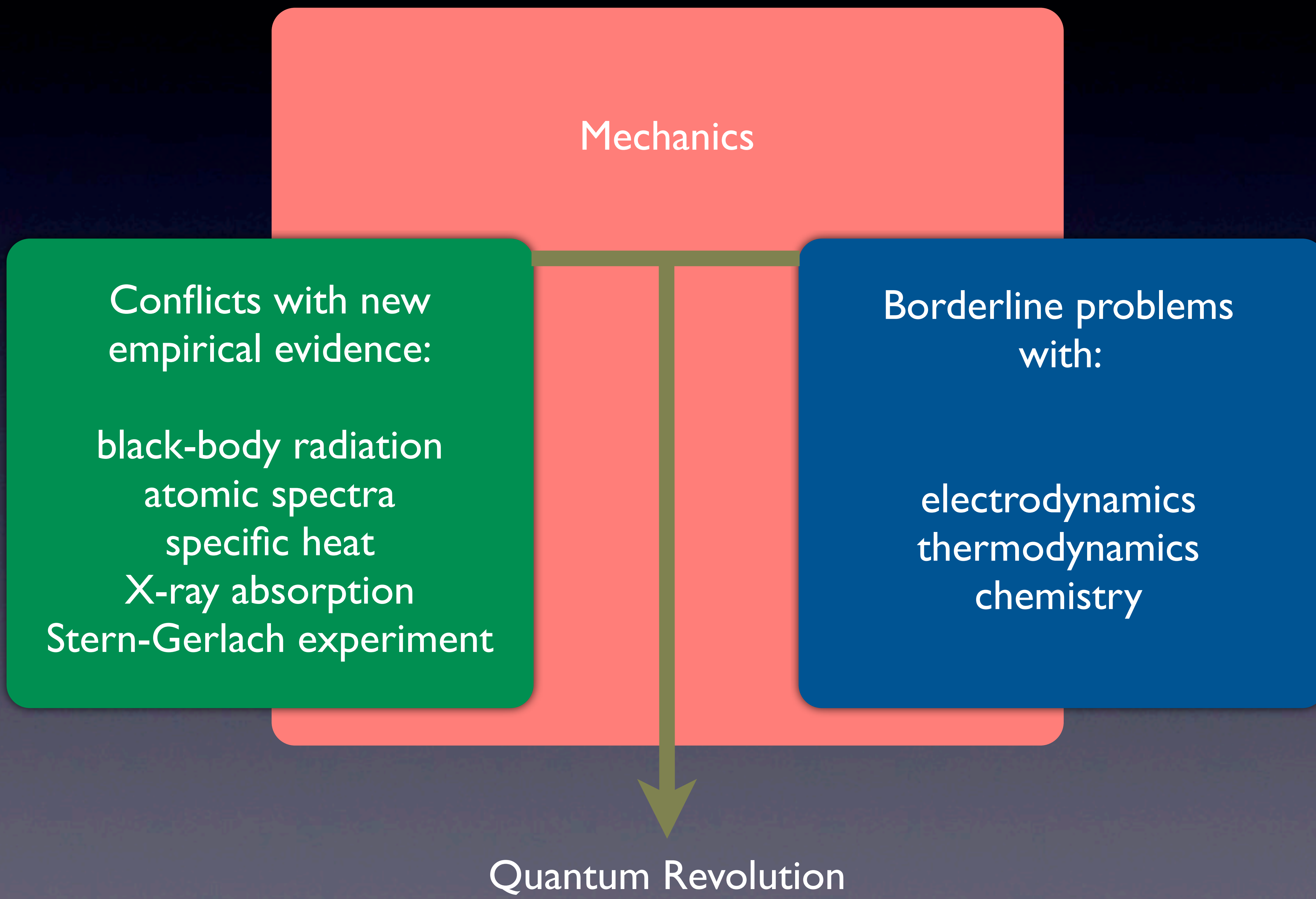


Albert Einstein (1879–1955)

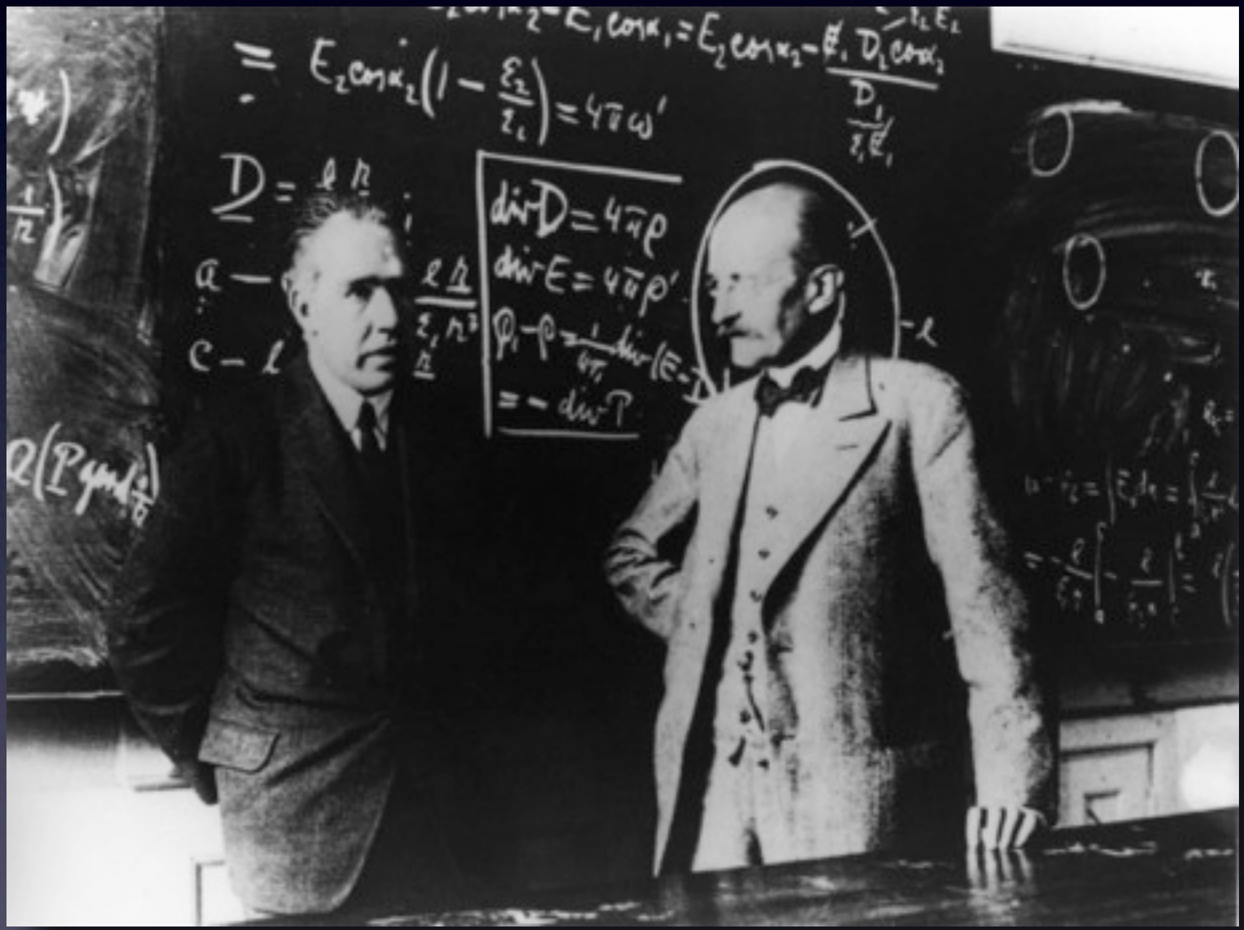
The Relativity Revolution

- In creating General Relativity Einstein pursued a double strategy.
- This heuristic strategy embodied a learning provess about how to integrate different elements of knowledge: the Newtonian limit, energy-momentum-conservation, the equivalence principle, the relativity principle
- His physical strategy started from candidate field equations for which the Newtonian limit was evident.
- His mathematical strategy started from candidate field equations whose covariance was evident.
- Was there anything in the quantum revolution corresponding to this double strategy?

The Origins of the Quantum Revolution



Historical Outline



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

19th century: emergence of the borderline problems

1900–1913: spread of insular quantum problems

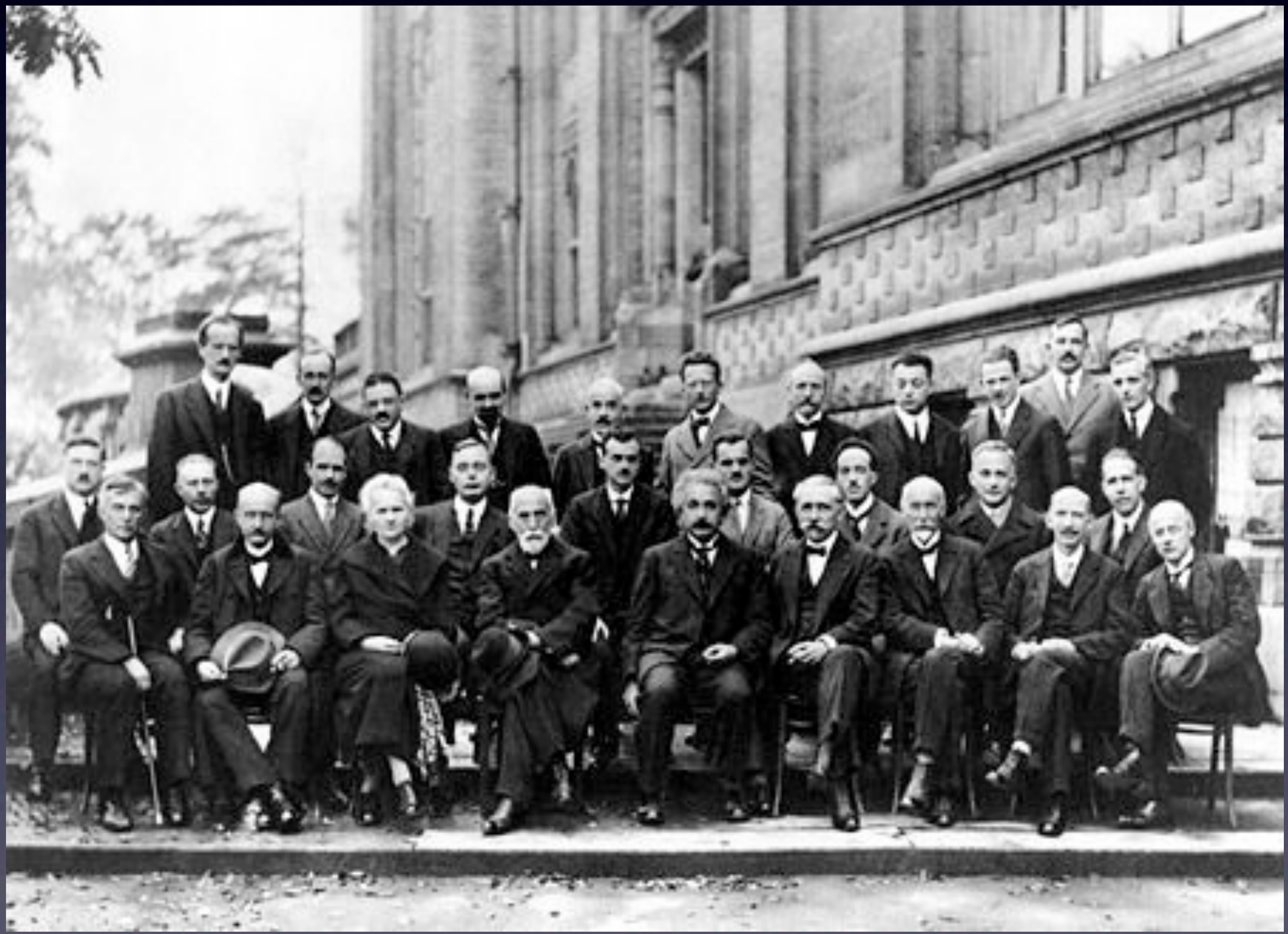
1913–1922: "old" quantum theory

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:

$$\oint p dq = nh$$

- **Correspondence principle:** The classical theory of electrodynamics offers a limit which restricts possible transitions between orbits.
- These were **heuristic schemes** rather than full-fledged theory.
- What were the crucial steps in the transition from old quantum theory to either matrix or wave mechanics?

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.
- Instead of a heuristic scheme, some physicists now sought for a “sharpened” formulation of the **correspondence principle** that would yield a full theory with the explanatory power to tackle the open problems.
- Heisenberg‘s 1925 **matrix mechanics** was an attempt to accomplish this using insights from the problems that troubled the old quantum theory (e.g., optical dispersion, multiplet structure).
- In 1926, Schrödinger‘s **wave mechanics**, however, offered an equally general theory, based on rather different evidence and principles.
- Very rapidly, it became clear that the two new theories are essentially **equivalent**.
- **How can this be?**

Part II:
Fraternal 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 equivalent in important respects?
- 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
- 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
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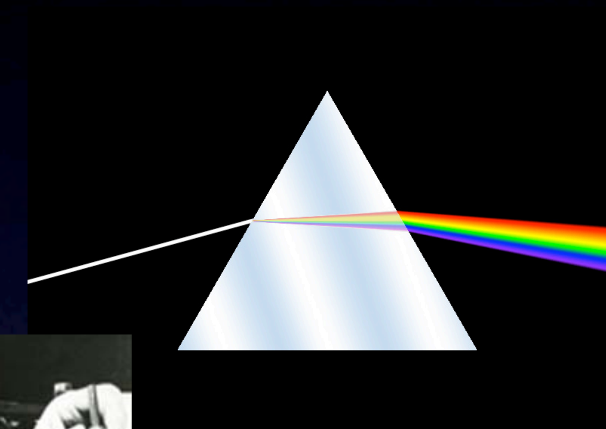
Optical Dispersion: Root of Matrix Mechanics

- **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

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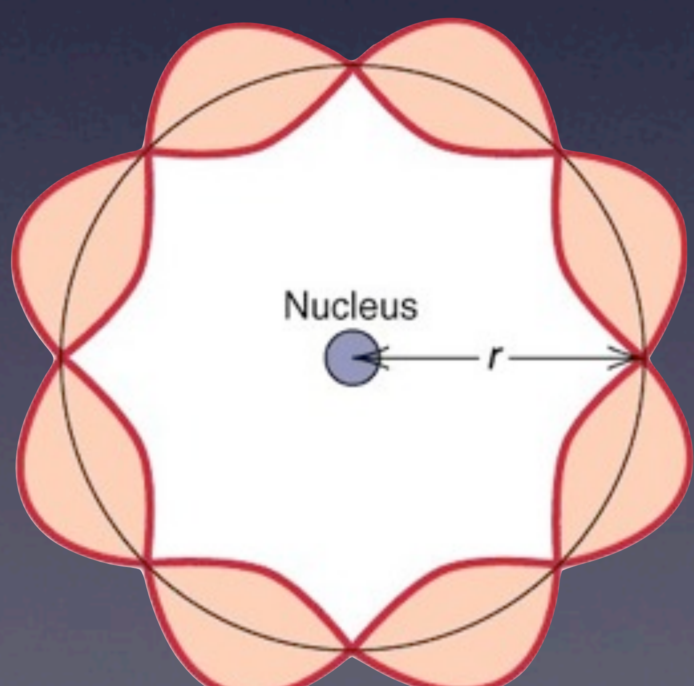
Gas Statistics and de Broglie‘s Matter Waves: Roots of Wave Mechanics

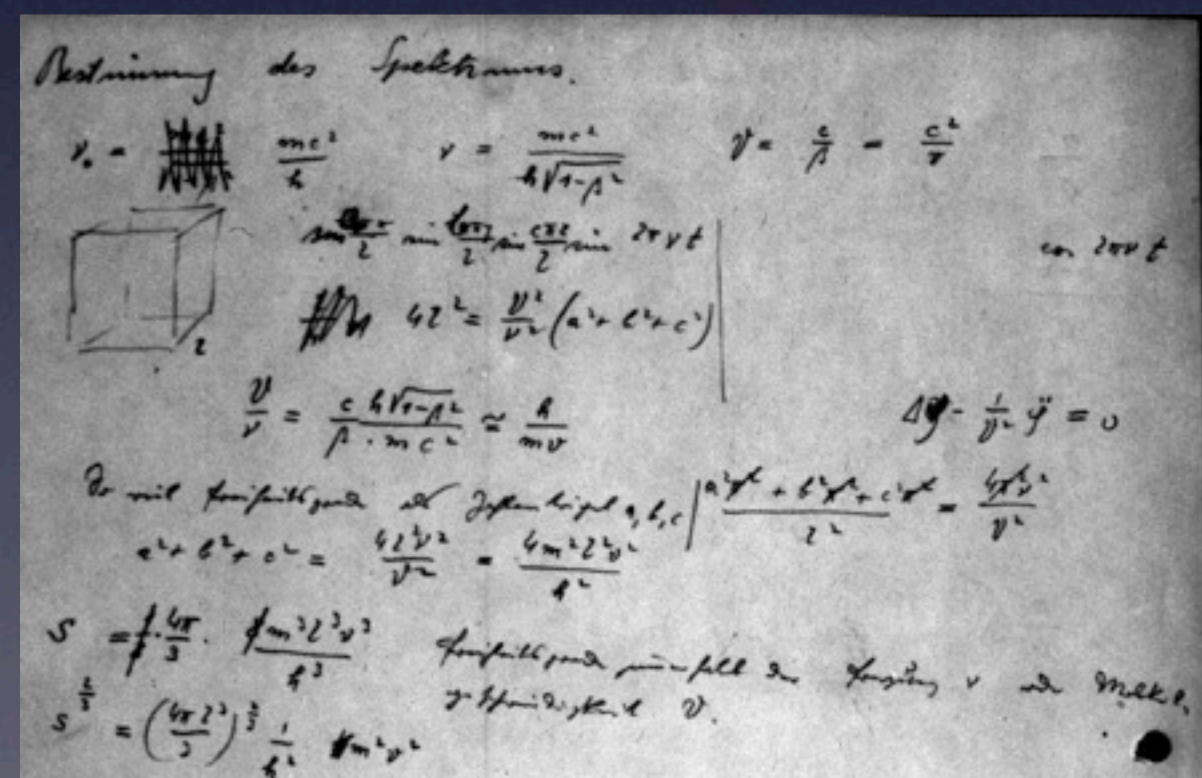
Schrödinger shows early interest in **"theoretical spectroscopy“** (1922 "On a Remarkable Property of Quantum Orbits of a Single Electron“)

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?
- Were both theories **incomplete** and did only their synthesis give rise to what we today know as quantum mechanics?
- Does reality enforce **convergence** of different theoretical approaches?
- Were pre-existing **mathematical structures**, such as the Hilbert space formalism, uncovered independently by the two approaches?

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, uncovered independently 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.)

Part III:
Classical Roots

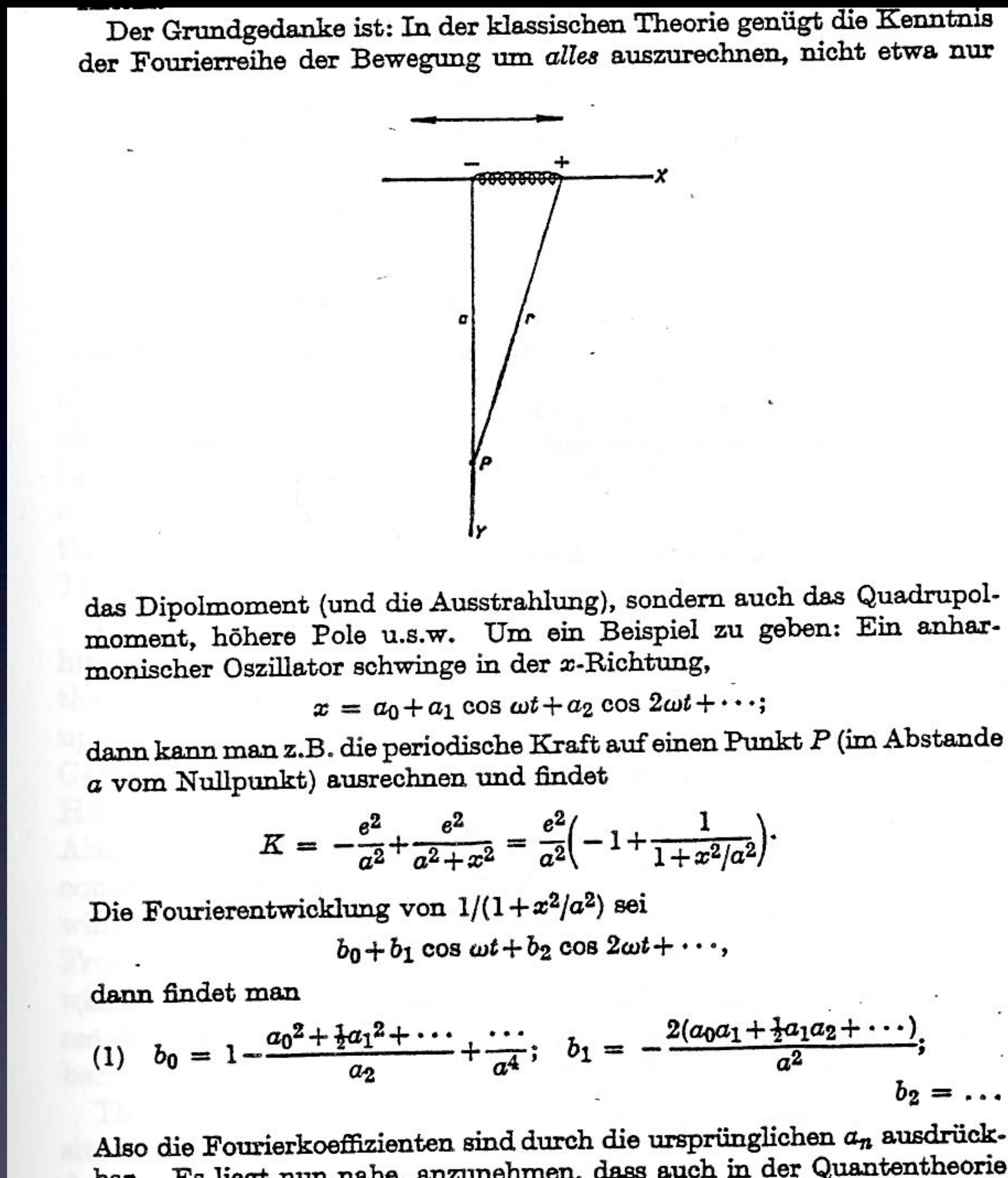
The Search for a “Sharpening” of the Correspondence Principle

- Around 1924, attempts were made to **“sharpen” the correspondence principle** into a general translation procedure allowing to derive quantum states from a classical description of physical systems.

- e.g., Born’s discretization of differential equations in his 1924 article “Über Quantenmechanik.”

- The successful application of virtual oscillators in the context of dispersion served as a hint that they might be a **model base different from classical orbits** for such a sharpened correspondence principle.

Heisenberg 1925: Umdeutung



Der Grundgedanke ist: In der klassischen Theorie genügt die Kenntnis der Fourierreihe der Bewegung um *alles* auszurechnen, nicht etwa nur das Dipolmoment (und die Ausstrahlung), sondern auch das Quadrupolmoment, höhere Pole u.s.w. Um ein Beispiel zu geben: Ein anharmonischer Oszillator schwinge in der x-Richtung,

$$x = a_0 + a_1 \cos \omega t + a_2 \cos 2\omega t + \cdots;$$

dann kann man z.B. die periodische Kraft auf einen Punkt P (im Abstande a vom Nullpunkt) ausrechnen und findet

$$K = -\frac{e^2}{a^2} + \frac{e^2}{a^2+x^2} = \frac{e^2}{a^2}\left(-1 + \frac{1}{1+x^2/a^2}\right).$$

Die Fourierentwicklung von $1/(1+x^2/a^2)$ sei

$$b_0 + b_1 \cos \omega t + b_2 \cos 2\omega t + \cdots,$$

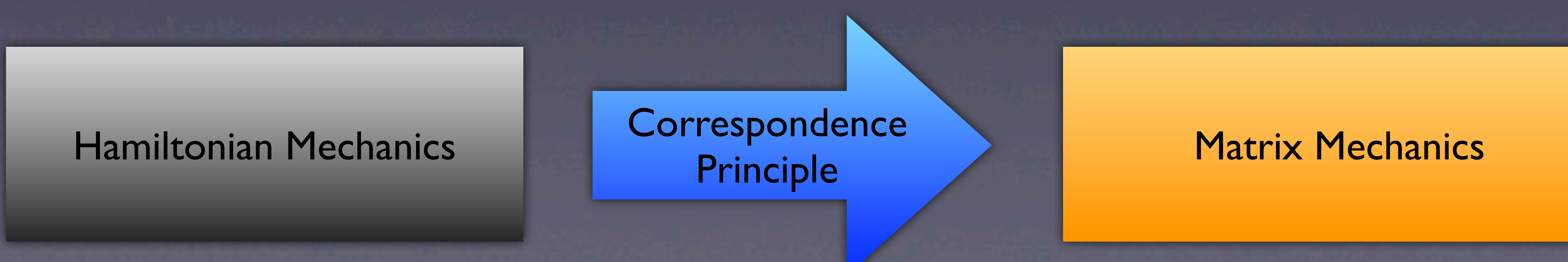
dann findet man

$$(1) \quad b_0 = 1 - \frac{a_0^2 + \frac{1}{2}a_1^2 + \cdots}{a_2} + \frac{\cdots}{a^4}; \quad b_1 = -\frac{2(a_0 a_1 + \frac{1}{2}a_1 a_2 + \cdots)}{a^2}; \quad b_2 = \ldots$$

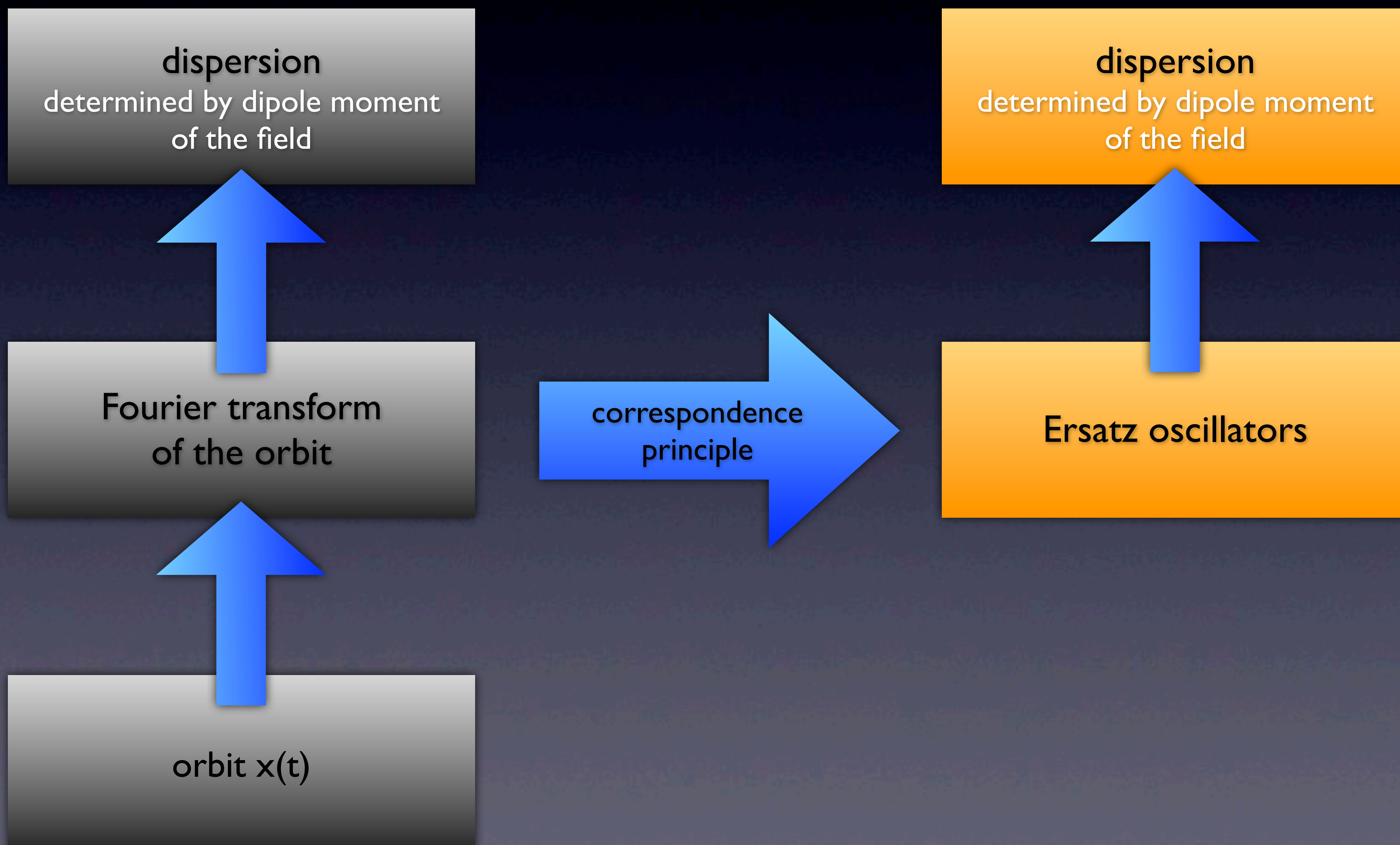
Also die Fourierkoeffizienten sind durch die ursprünglichen a_n ausdrückbar. Es liegt nun nahe, anzunehmen, dass auch in der Quantentheorie

"The basic idea is: In the classical theory, knowing the Fourier expansion of the motion is enough to calculate **everything**, not just the dipole moment (and the emission), but also the quadrupole of higher moments, etc."

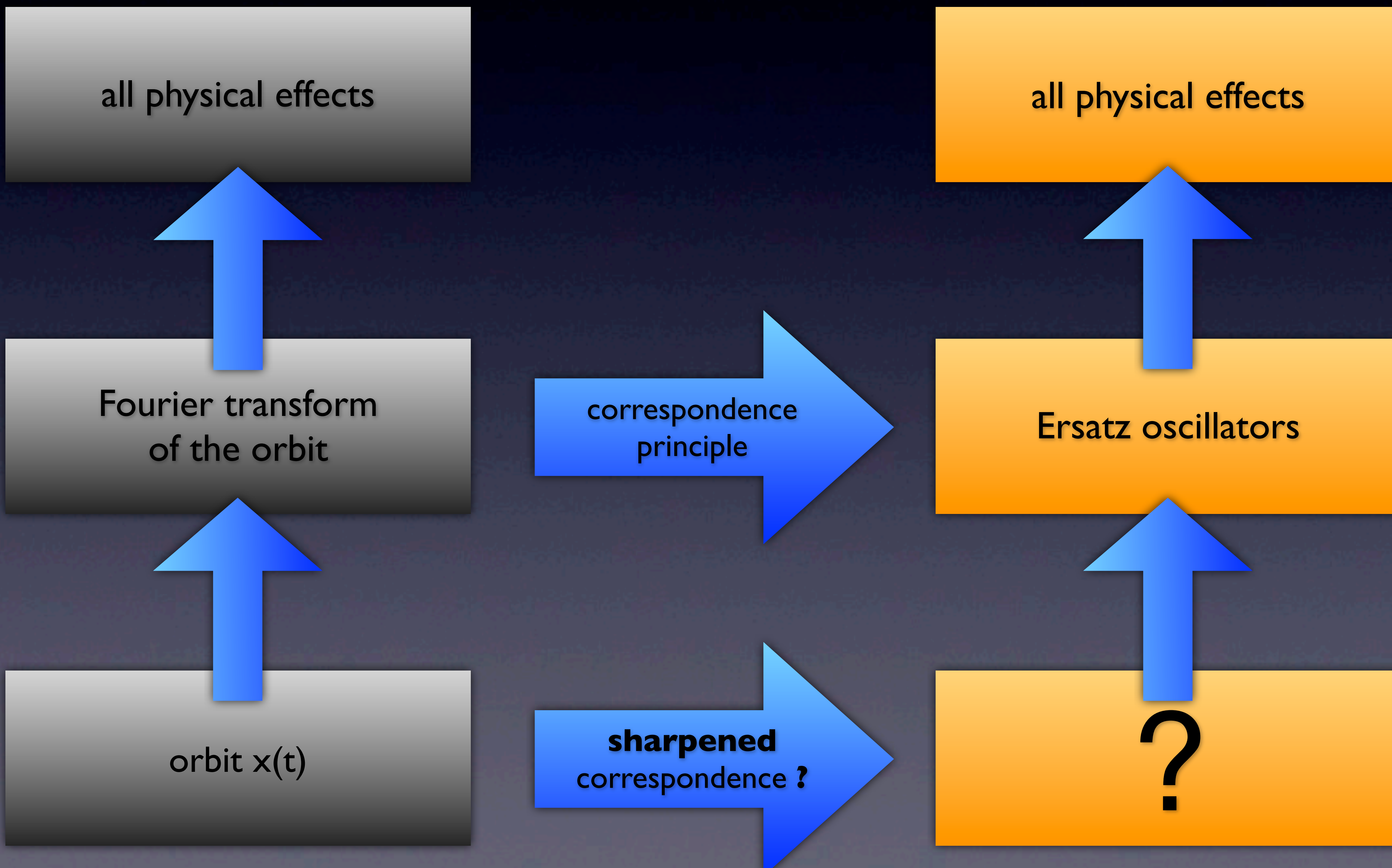
Heisenberg to Kronig, May 1925



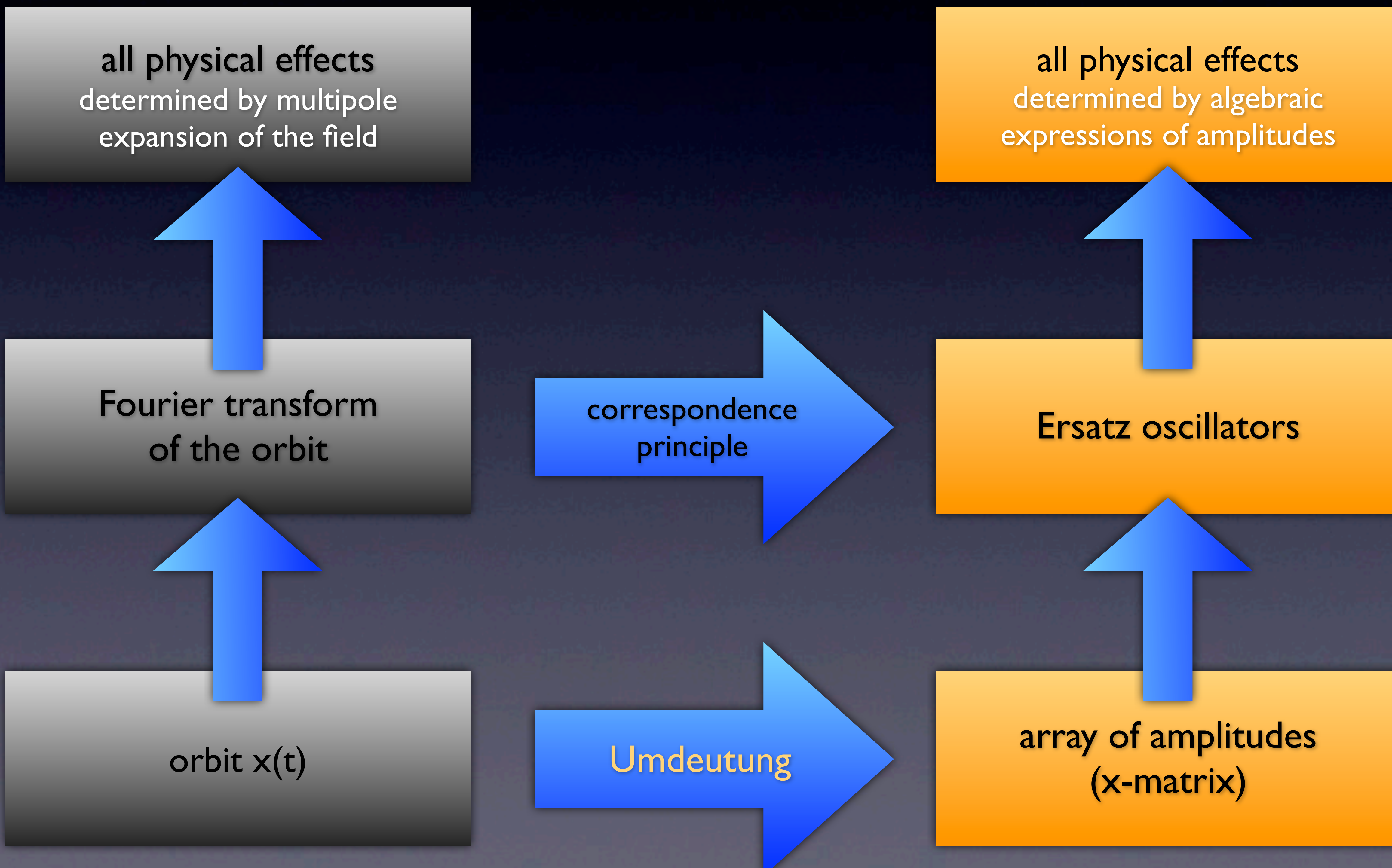
Heisenberg, Kramers (Jan. 1925): Dispersion Theory



The Search for the Sharpened Correspondence Principle



Heisenberg (July 1925): Umdeutung



Heisenberg's Re-Casting of the Correspondence Principle

Die Antwort lautet klassisch offenbar so:

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

bzw.

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

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

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

bzw.

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

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

Heisenberg, Umdeutung (1925)

Heisenberg‘s Re-Casting of the Correspondence Principle

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

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:

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

das heißt

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

Heisenberg's Re-Casting of the Correspondence Principle

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

$$h = 4\pi m \sum_{0}^{\infty} \alpha \left\{ |a(n, n+\alpha)|^2 \omega(n, n+\alpha) - |a(n, n-\alpha)|^2 \omega(n, n-\alpha) \right\}, \quad (16)$$

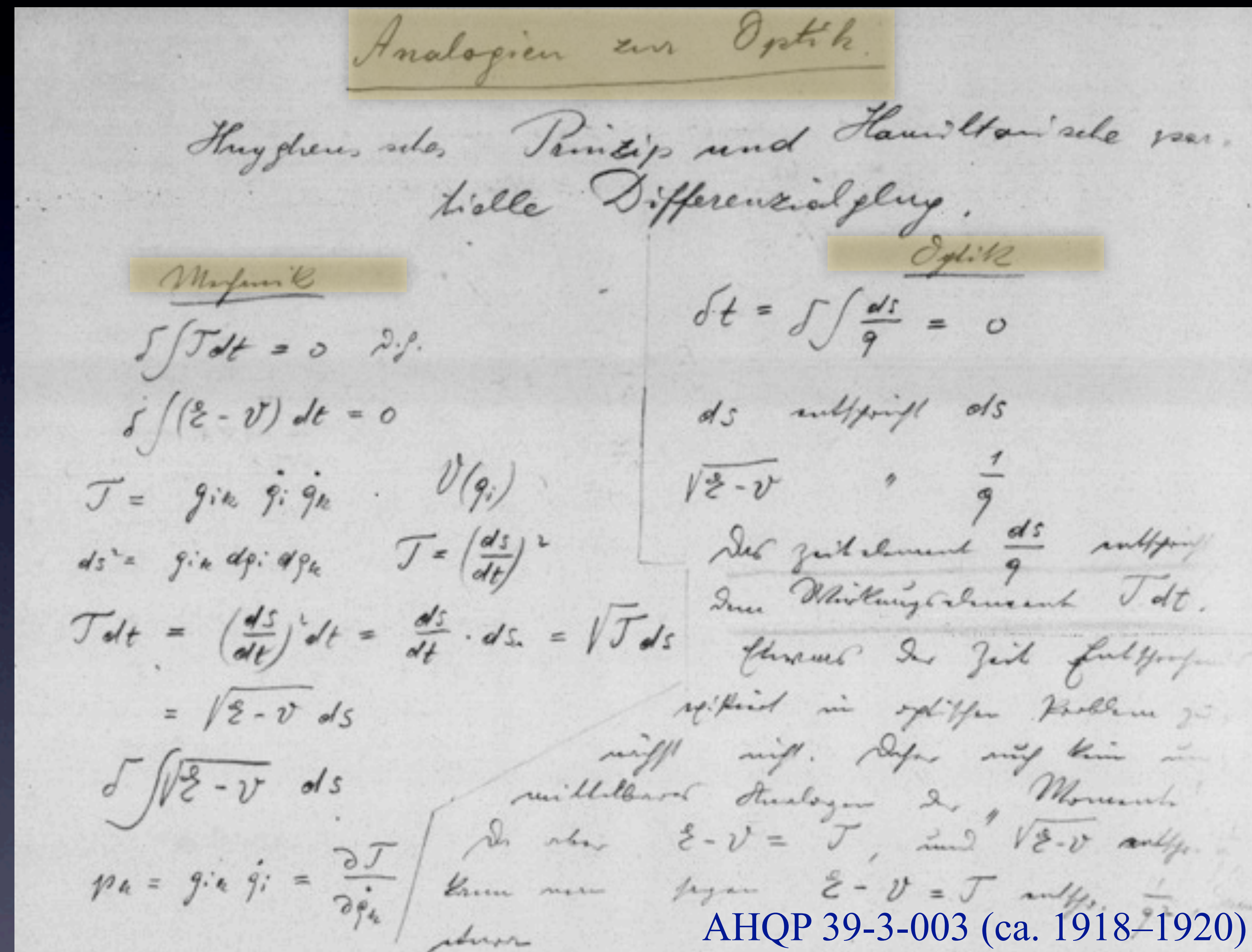
doch diese Beziehung genügt hier zur eindeutigen Bestimmung der a; denn die in den Größen a zunächst unbestimmte Konstante wird von selbst durch die Bedingung festgelegt, daß es einen Normalzustand geben solle, von dem aus keine Strahlung mehr stattfindet; sei der Normalzustand mit n_0 bezeichnet, so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

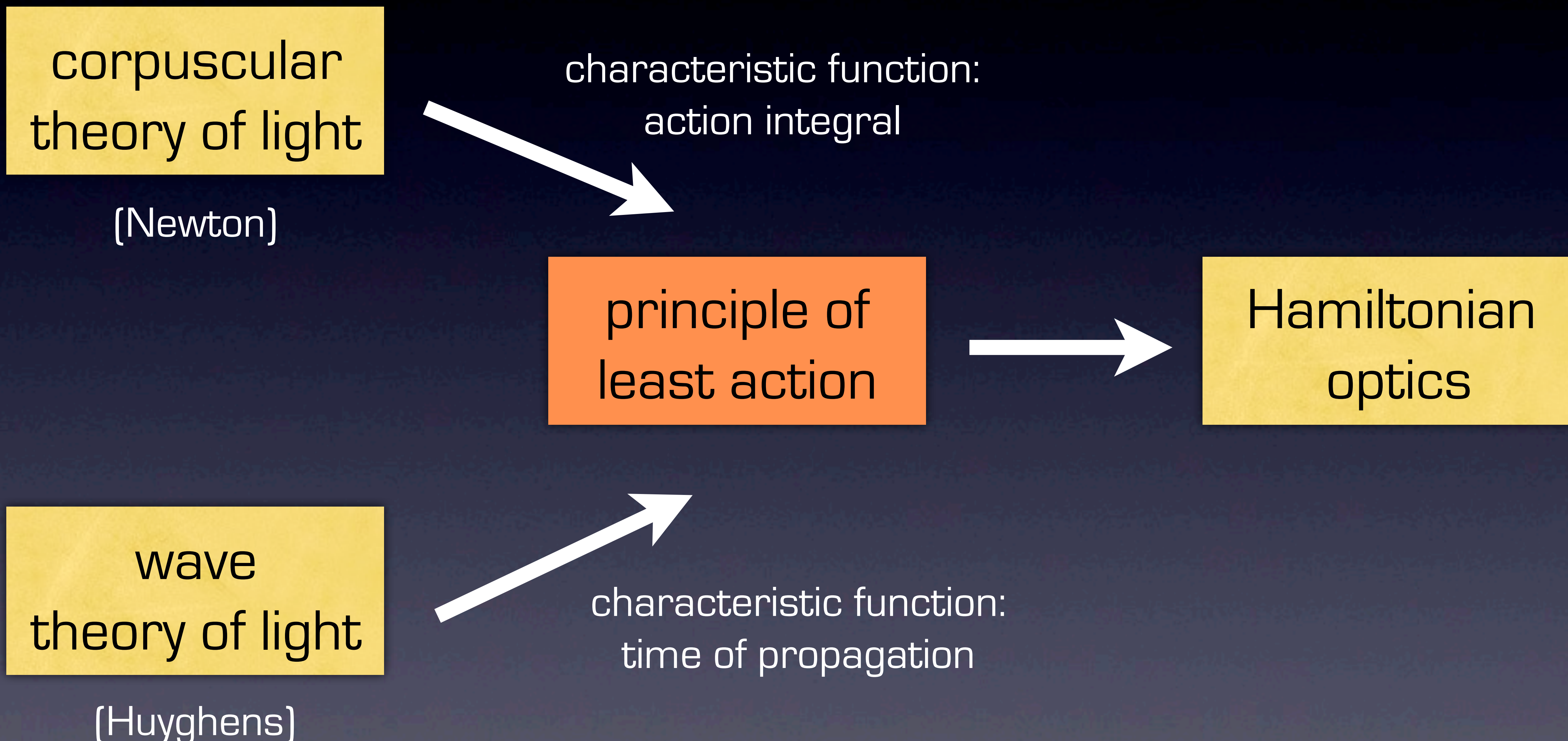
Schrödinger's Completion of Hamilton's Analogy

- 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).

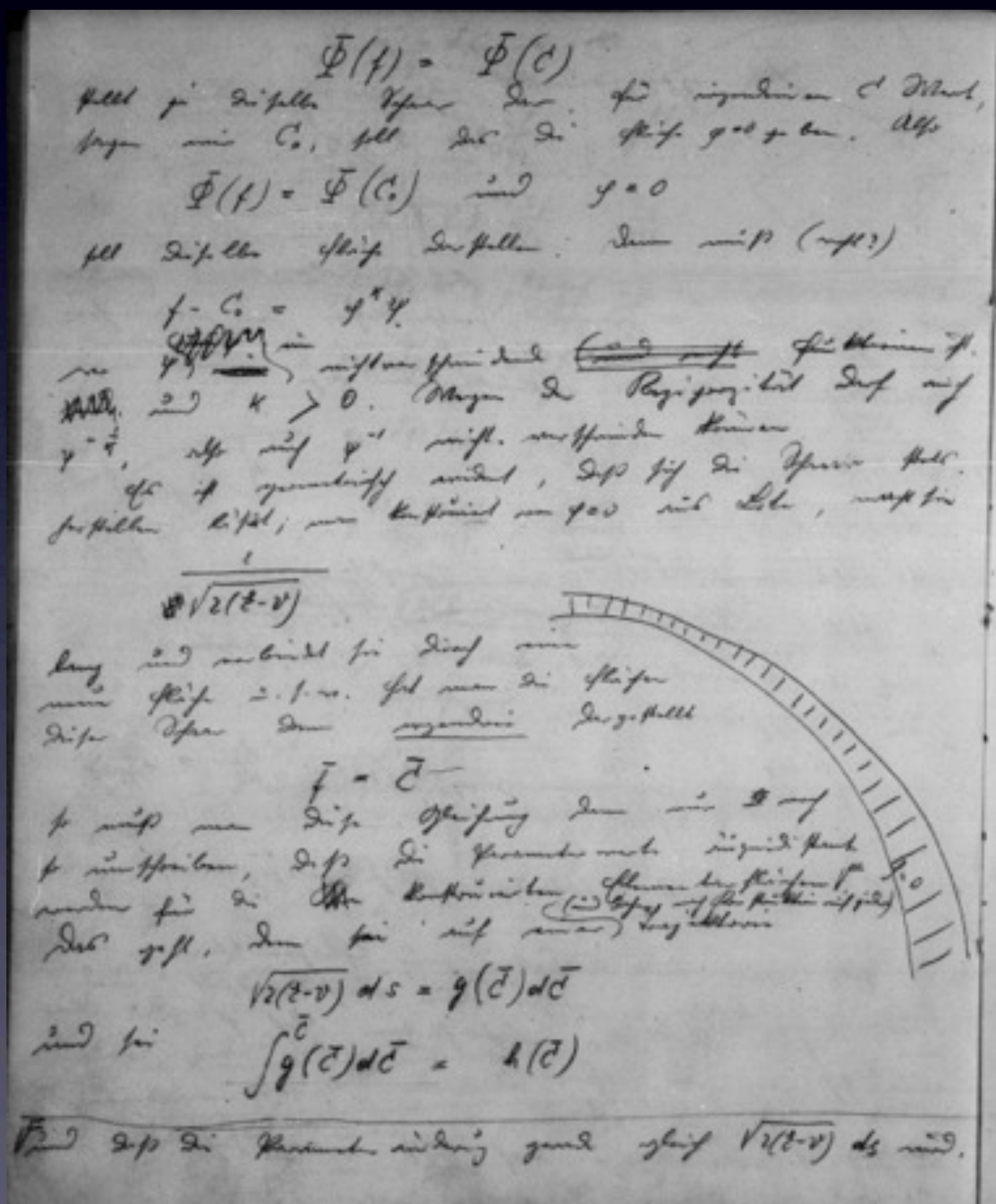
Schrödinger’s Completion of Hamilton’s Analogy: Hamiltonian Optics



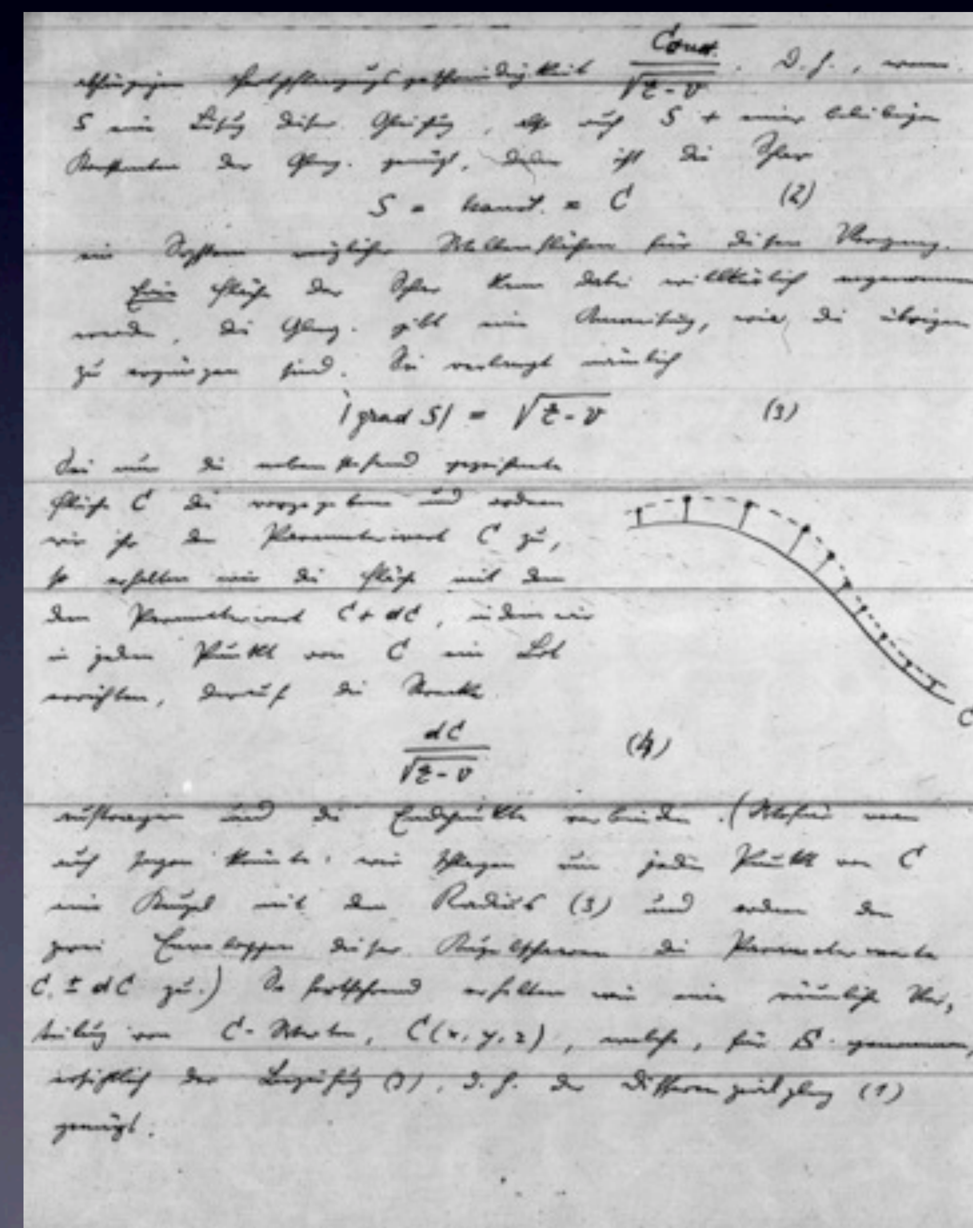
guiding motivation: cast geometrical or “ray” optics into a general scheme having the "power and dignity ... of the general method of Lagrange" so fruitful in mechanics

Schrödinger’s Completion of Hamilton’s Analogy

Reappearance of the analogy in 1925-1926 notebooks

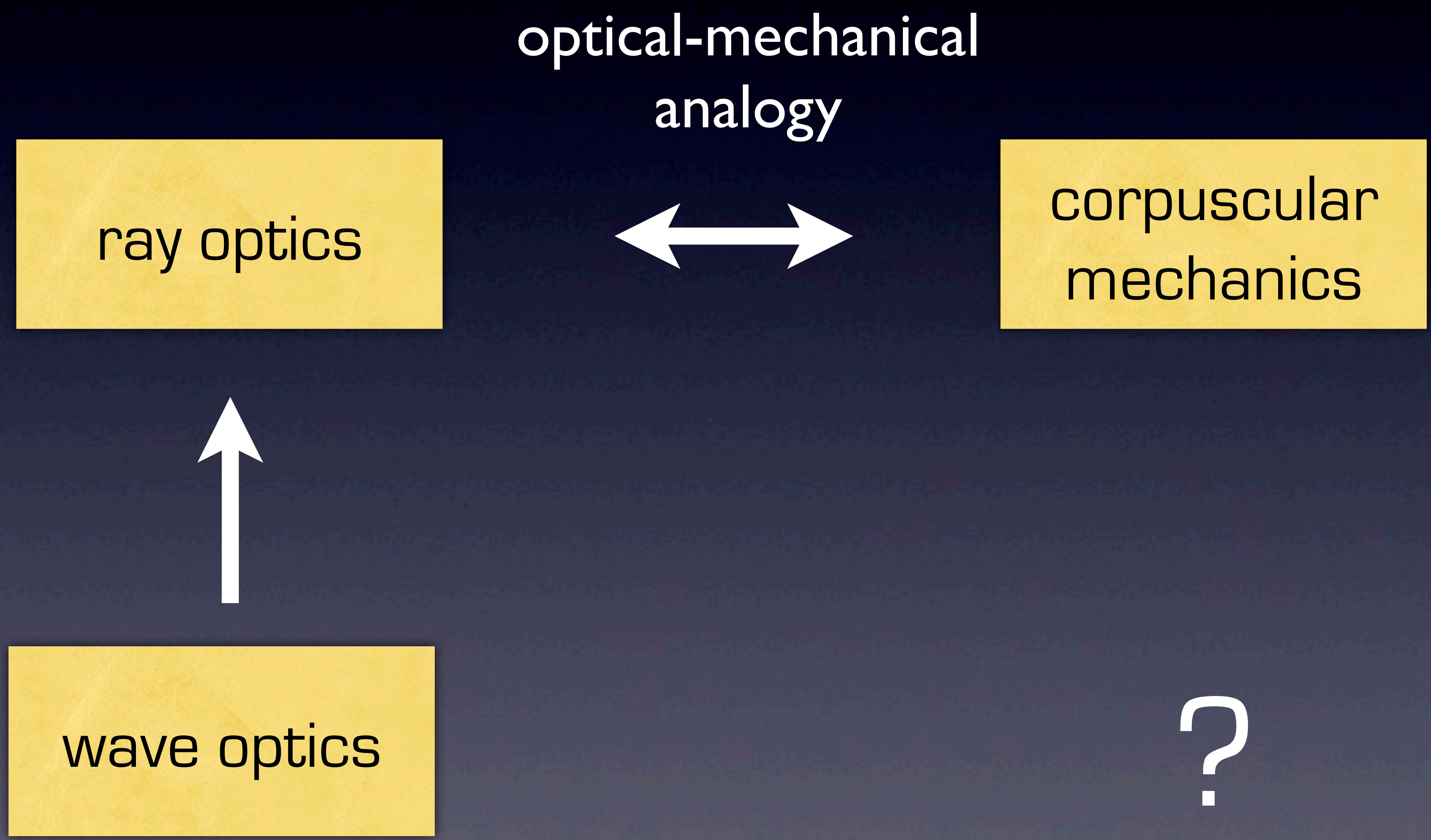


Notebook ”Tensor-Analytic Mechanics“
AHQP 39-3-001 (ca. 1918–1920)

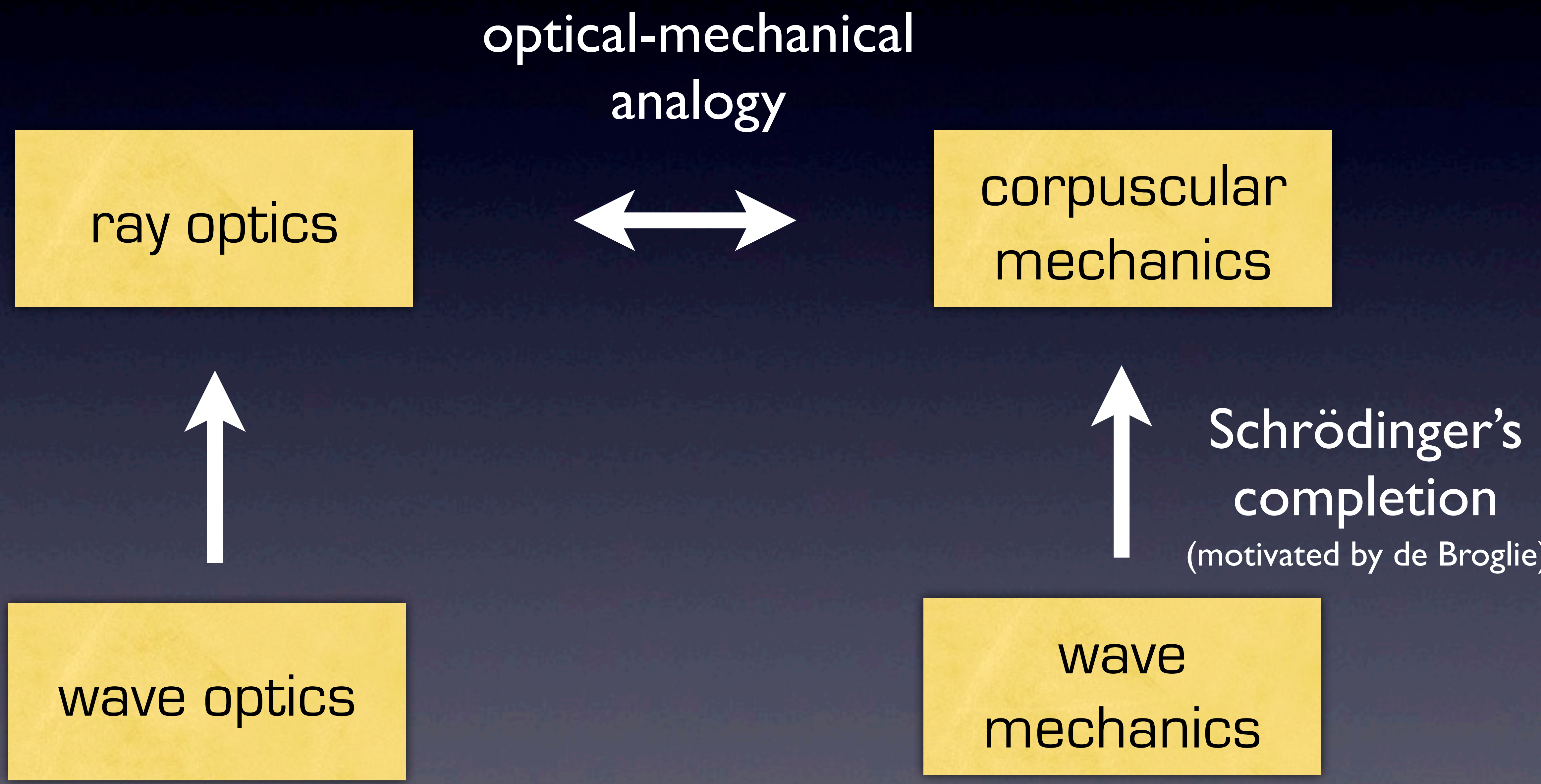


Notebook “Eigenvalue Problem of the Atom II.“
AHQP 40-6-001 (ca. Feb. 1926)

Schrödinger's Completion of Hamilton's Analogy



Schrödinger's Completion of Hamilton's Analogy



Old quantum theory is the limiting case of a more general wave mechanics!

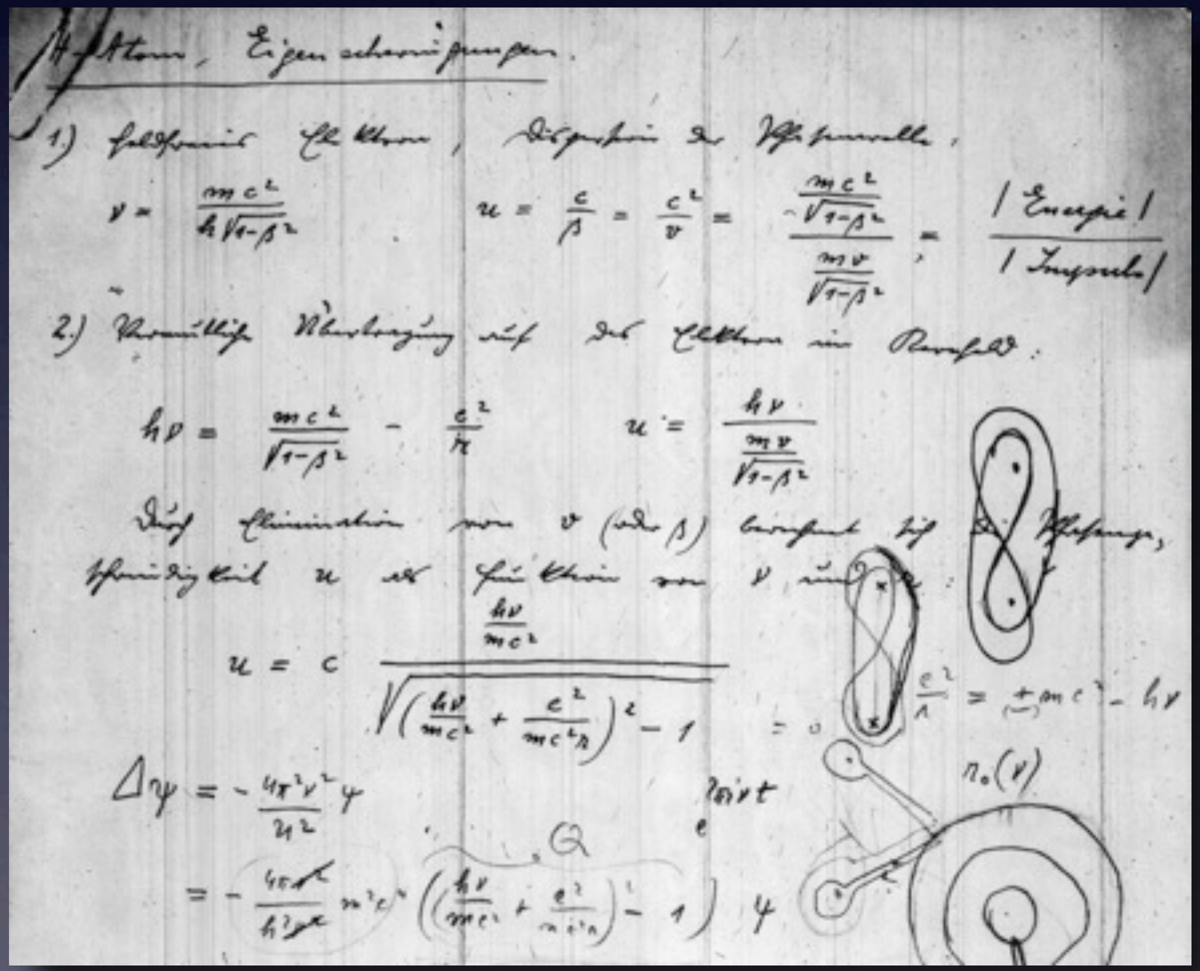
Schrödinger's Completion of Hamilton's Analogy

- 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**

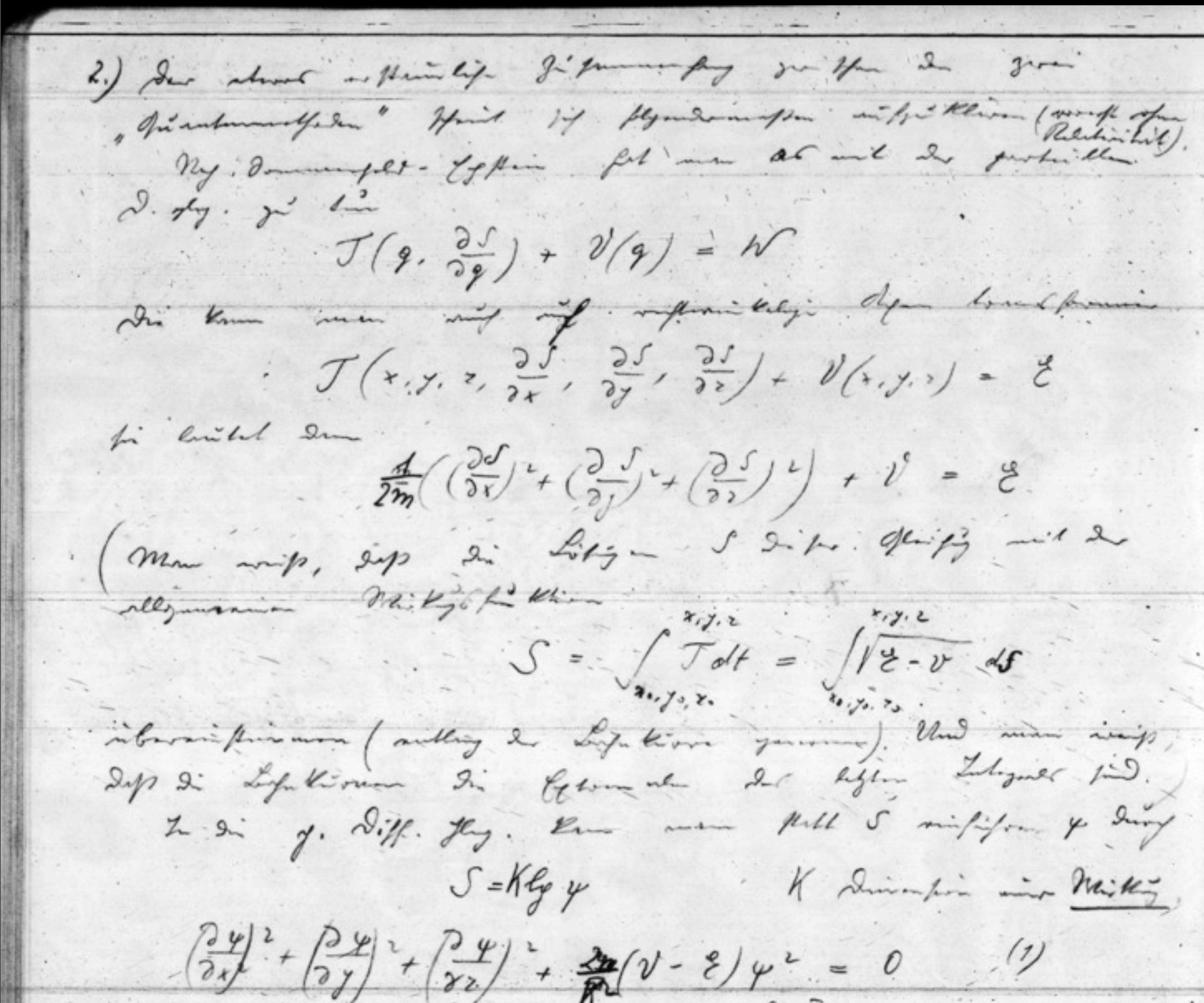
- Through the optical-mechanical analogy, he gets the correspondence principle „for free".



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

Schrödinger's Completion of Hamilton's Analogy

Confrontation with the old quantum theory:



$$T\left(q, \frac{\partial S}{\partial q}\right) + V(q) = W$$

$$T\left(x, y, z, \frac{\partial S}{\partial x}, \frac{\partial S}{\partial y}, \frac{\partial S}{\partial z}\right) + V(x, y, z) = E$$

$$\frac{1}{2m}\left(\left(\frac{\partial S}{\partial x}\right)^2 + \left(\frac{\partial S}{\partial y}\right)^2 + \left(\frac{\partial S}{\partial z}\right)^2\right) + V = E$$

$$S = \int_{x_0, y_0, z_0}^{x, y, z} T\,dt = \int_{x_0, y_0, z_0}^{x, y, z} \sqrt{E - V}\,ds$$

$$S = K \lg \psi$$

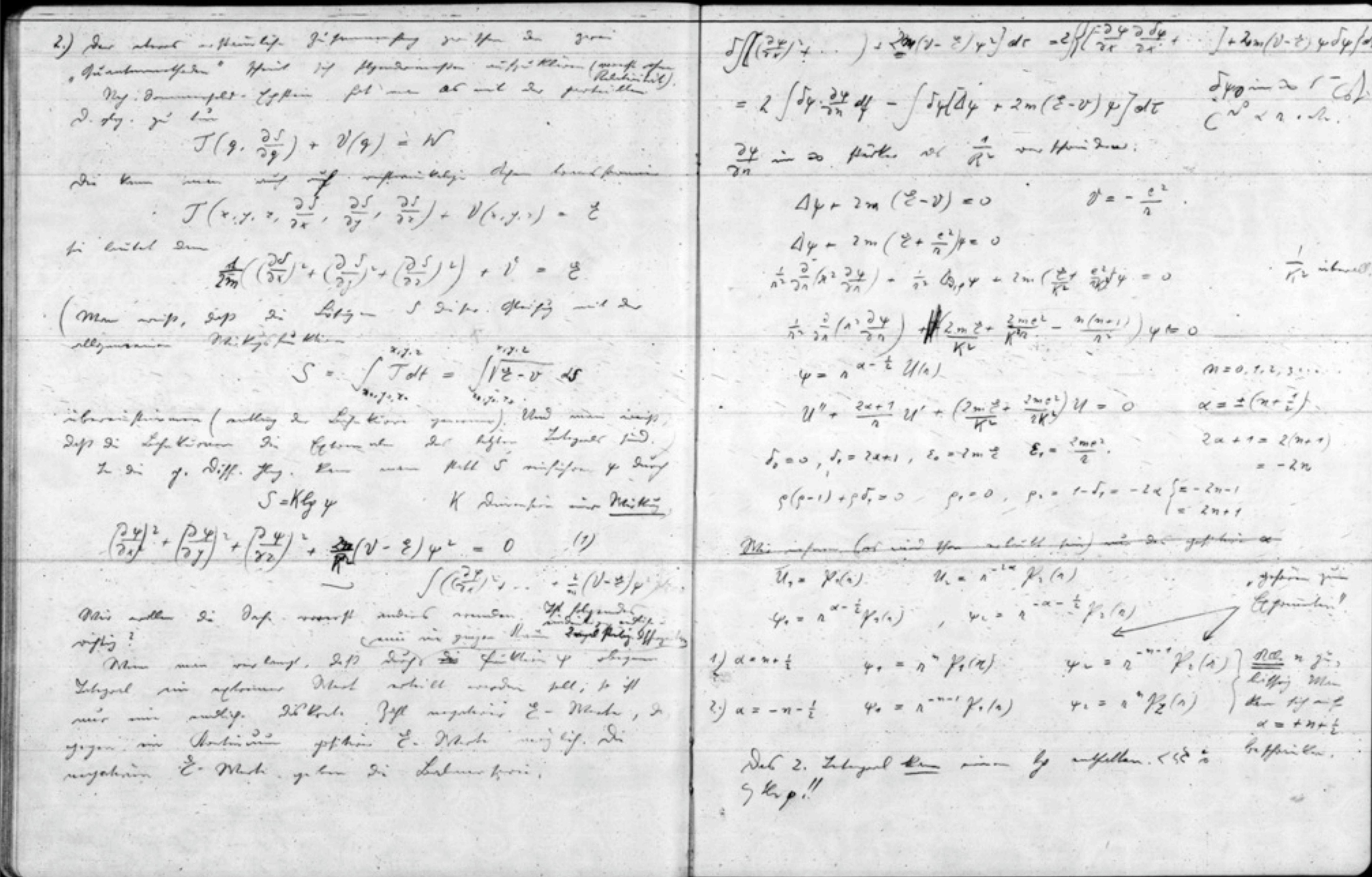
$$\left(\frac{\partial \psi}{\partial x}\right)^2 + \left(\frac{\partial \psi}{\partial y}\right)^2 + \left(\frac{\partial \psi}{\partial z}\right)^2 + \frac{2m}{K^2}(V - E)\psi^2 = 0 \quad (1)$$

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

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

Schrödinger's Completion of Hamilton's Analogy

Confrontation with the old quantum theory:



Conclusion: Pre-established Harmony?
The Genetic View:

- Both theories are transformations of a **common ancestor**: old quantum theory!
- Both theories **preserve** the formal structure of Hamiltonian mechanics.
- Both theories involve a **translation procedure** connecting classical with quantum concepts.
- Both theories incorporate the **new knowledge** about the energy-frequency condition.