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

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Abstract

The optical-mechanical analogy played a central role in Schrödinger's reception of de Broglie's ideas and development of wave mechanics. He was well acquainted with it through earlier studies, and it served him as a heuristic model to develop de Broglie's idea of a matter wave. Schrödinger's struggle for a deeper understanding of the analogy in the search for a relativistic wave equation led to a fundamental transformation of the role of the analogy in his thinking into a formal constraint on possible wave equations. This development strongly influenced Schrödinger's interpretation of the wave function and helps to understand his commitment to a wave interpretation in opposition to the emerging mainstream. The changes in Schrödinger's use of the optical-mechanical analogy can be traced in his research notebooks, which offer a much more complete picture of the development of wave mechanics than has been generally assumed. The notebooks document every step in the development and give us a picture of Schrödinger's thinking and aspirations that is more extensive and more coherent than previously thought possible.

Key words: quantum mechanics, wave mechanics, Hamilton, W. R., Schrödinger, E., optical-mechanical analogy

1. The roots of wave mechanics

The genesis of wave mechanics has been treated by many authors. In a first stage, these studies relied mostly on Erwin Schrödinger's published works and reminiscences of his colleagues (Klein, 1964; Gerber, 1969; Kubli, 1970). These accounts have been substantially revised by historians who also considered the existing correspondence (Raman and Forman, 1969; Hanle, 1971, 1977, 1979; Wessels, 1979). The various authors mentioned above have drawn different

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conclusions about the roots, the trajectory, and the goals of Schrödinger's project on wave mechanics, which we will discuss in more detail below. However, in the years from 1925–1927, Erwin Schrödinger wrote, besides his well-known four communications on wave mechanics (Schrödinger, 1926b,c,e,f) and several other relevant publications (e. g., Schrödinger, 1926d) dozens of notebooks comprising hundreds of pages. These notebooks are an obvious source for a more detailed understanding of his work and his ambitions in the years of the creation of wave mechanics. Yet, Schrödinger's notebooks have only been discussed in some detail by Kragh (1982, 1984) and Mehra and Rechenberg (1987a,b) who found various tantalizing passages from the notebooks relevant for the discussion.

Complementing the study of these passages with an analysis of a larger set of notebooks, we arrive at a rather coherent picture of Schrödinger's motivations and thought development through the creation of wave mechanics. Therefore, we cannot agree with the assessment that "Schrödinger has left few traces of how his ideas evolved as he worked towards wave mechanics" (Wessels, 1979), which is frequently found in the older literature on the subject. We have studied 27 notebooks contained in the AHQP that we identified as possibly stemming from the period of the development of wave mechanics as well as some earlier notebooks and manuscripts that have long been known (Raman and Forman, 1969) to be important for the prehistory of Schrödinger's program (see Fig. 1).[1]

Already Klein (1964), and later Hanle (1971), pointed out that an important root of the development of wave mechanics is Schrödinger's interest in gas statistics in 1924–1925. It was in this context that Schrödinger encountered Albert Einstein's paper "Quantentheorie des einatomigen idealen Gases" (Einstein, 1924) which used Bose statistics to derive a state function of the ideal gas. Einstein mentioned that Louis de Broglie's idea of matter waves could help to make understandable the physical content of the Bose-Einstein statistics. In the fall of 1925, instigated by this remark, Schrödinger studied de Broglie's thesis. In his paper "Zur Einsteinschen Gastheorie" (Schrödinger, 1926a) he pointed out that the Bose-Einstein counting procedure, which seems rather *ad hoc* as a counting method for particles, can be understood as a straightforward Boltzmann counting method for standing wave modes (Schrödinger called this "natural statistics"). This is an obvious starting point in his development of a wave equation for matter waves.

Raman and Forman (1969) favor an alternative explanation for Schrödinger's interest in de Broglie's idea of matter waves. They point to a paper from 1922, "Über eine bemerkenswerte Eigenschaft der Quantenbahnen eines einzelnen Elektrons" (Schrödinger, 1922), which uses an argument similar to de Broglie's to derive Bohr's quantized orbits. Although Schrödinger's argument does not follow from a context of matter waves but rather was inspired by his study of Weyl's unified field theory, Raman and Forman argue that the formal parallel between de Broglie's and Schrödinger's own work made him receptive to de Broglie's ideas. Even though Raman and Forman are able to support this argument by some elements from Schrödinger's correspondence, there is no evidence for a continuing interest of Schrödinger's along the lines of this paper in the years 1922–1925.

Kragh (1982) as well as Mehra and Rechenberg (1987a,b) consider a third explanation for Schrödinger's interest in de Broglie. De Broglie's use of the formal analogy between Fermat's

[1]The notebooks are reproduced in the Archive for the History of Quantum Physics (AHQP) available on microfilm in several institutions (original repository: American Philosophical Society, Philadelphia). They will be quoted by their AHQP reel and document numbers, as shown in Fig. 1. The AHQP dating is incorrect for some of the notebooks, especially for the early and later ones (so is, e. g., 41-2-001 clearly written before (Schrödinger 1926d)). However, since the evidence is rather ambiguous in many cases, we will not attempt to give dates for all the notebooks in the list, but will only discuss in the text the dating for the notebooks that we treat in more detail.

AHQP	Title	AHQP dating
39-3-001	Tensoranalytische Mechanik I	apparently ca. 1914
39-3-002	Tensoranalytische Mechanik II	apparently ca. 1914
39-3-003	Tensoranalytische Mechanik III & Optik inhomogener Medien	apparently ca. 1914
39-3-004	Hertz'sche Mechanik und Einstein'sche Gravitationstheorie	perhaps ca. 1915
39-3-005	*untitled manuscript draft continuing the previous one*	perhaps ca. 1915
40-5-001	Unidentified notes on electromagnetic(?) waves	1925/1926
40-5-002	H-Atom — Eigenschwingungen	evidently late 1925 or Jan. 1926
40-5-003	Eigenwertproblem des Atoms. I.	evidently late 1925 or Jan. 1926
40-6-001	Eigenwertproblem des Atoms. II.	evidently ca. Feb. 1926
40-6-002	Starkeffekt fortgesetzt	probably ca. Feb. 1926
40-7-001	Summen von Binomialen. Eigenwertproblem d. Atoms. III.	evidently ca. Mar. 1926
40-7-002	Berechnung der Hermiteschen Orthogonalfunktionen	probably early 1926
40-7-003	Loose notes on intensities, transition probabilities	probably 1926
40-8-001	Intensitätsberechnung für den Starkeffekt	evidently spring 1926
40-9-001	Einstein-Planck-Statistik [durchgestrichen]	evidently ca. 1926
41-1-004	Kugelmethode auf Dirac- und Gordongl. angew.	perhaps early 1927
41-1-001	Dirac. Nebenbedingungen.	perhaps mid 1926
41-1-002	Undulatorische Statistik I.	perhaps late 1926
41-1-003	Undulatorische Statistik II.	perhaps early 1927
41-2-001	Intensitäten. Parallele zu Heysenberg und Lanczos	perhaps 1927
41-2-002	Die schwebenden Fragen.	perhaps 1927
41-2-004	Streckenspektrum, Intensitäten	perhaps 1927
41-2-005	Studien über Integralgleichungen und Kerne.	3 May 1927
41-4-001	Koppelung. Ganz alt.	perhaps 1927
41-4-002	Allgemeine Dispersionstheorie, Kopplung II.	perhaps 1927
41-4-003	Koppelung mit dem Strahlungsfeld.	probably late 1927
41-4-004	Dispersion und Resonanz	June 1928
41-4-005	Berlin 1928	1928
41-4-006	Funkenwahrscheinlichkeit	June 1928
41-5-001	Darstellungen	perhaps 1928
41-5-002	Zur Abel'schen Integralgleichung	perhaps 1928
41-2-003	Zu unscharfe Spektren	perhaps 1927

Figure 1: Possibly relevant notebooks from Schrödinger's nachlass. First column: AHQP Film-Section-Item; second column: Schrödinger's title; third column: dating according to AHQP.

principle for ray optics and Maupertuis' principle for corpuscular mechanics appealed to Schrödinger because of his own explorations of Hamiltonian mechanics around 1920 which had led him to study Hamilton's optical-mechanical analogy. Three notebooks titled "Tensoranalytische Mechanik", tentatively dated to 1918–1922,[2] deal with an extension of classical mechanics inspired by Albert Einstein's recently published theory of general relativity and by Heinrich Hertz's reformulation of classical mechanics in differential geometrical form, presented in *Die Prinzipien der Mechanik in neuem Zusammenhange dargestellt* (Hertz, 1894). In the second of these notebooks, Schrödinger explored Hamilton's optical-mechanical analogy in a section titled "Analogien zur Optik" (see Fig. 3).[3] The optical-mechanical analogy was prominently used by

[2]There is very little hard evidence for the dating of these notebooks. For the lower bound we use Schrödinger's mention of (Weyl, 1918) in the second notebook, for the upper bound the assumption that the notebooks were written before (Schrödinger, 1922), which uses Weyl's gauge theory that is not mentioned in the notebooks.

[3]The notebooks are also mentioned by Raman and Forman (1969), but not considered as very important in their argument.

Schrödinger in his second communication on wave mechanics as a heuristic justification, but there has been considerable debate how much of a role it played in the actual process of discovery.

In this paper, we want to show that all these seemingly disparate roots of Schrödinger's interest in wave mechanics are substantially interconnected in his thinking. From the study of Schrödinger's notebooks, it becomes clear that they all were different facets of his longstanding interest in extending classical mechanics, inspired equally by 19th century analytical mechanics, Boltzmann's statistical mechanics, Einstein's General Relativity, and the problem of a physical understanding of the old quantum theory. The Hamiltonian analogy became the most fruitful piece in this complex network of theoretical speculation. During the development of wave mechanics, for Schrödinger both the content and the use of the analogy changed considerably. We will trace these developments through Schrödinger's notebooks from the time of the First World War to 1926.

2. Hamilton's optical-mechanical analogy

The optical-mechanical analogy goes back to William Rowan Hamilton (Hamilton, 1833).[4] It was mostly ignored during the 19th century but reached considerable prominence with the development of wave mechanics. In this section, we will consider its original formulation and the history of its reception through the 19th century.

Hamilton's early work was mostly devoted to ray optics. In the 1820s, neither Newton's emission theory of light nor Huyghens' wave theory were unanimously accepted. Hamilton himself became a vigorous defender of wave optics, but in his work on geometrical optics he was not concerned with questions about the nature of light but treated ray optics as a purely geometrical problem.[5] Hamilton's treatment starts from a generalization of Malus's theorem: for any bundle of light rays emitted from a point, there will be a family of surfaces so that all light rays are orthogonal to these surfaces. Hamilton shows that Malus's theorem holds in full generality also for inhomogeneous and anisotropic media, and that the family of surfaces can be described by a potential function, the characteristic function (i. e., the surfaces are the surfaces of constant value of the function). This function can be found through solving a partial differential equation, the Hamiltonian partial differential equation, which will be of central importance for our story. The characteristic function gives a complete description of an optical system of rays, such as in an optical apparatus. Thus, Hamilton is able to formulate a theory of ray optics that is as general as the Lagrange theory of mechanics:

> Those who have meditated on the beauty and utility, in theoretical mechanics, of the general method of Lagrange—who have felt the power and dignity of that central dynamical theorem which he deduced, in the *Mécanique Analytique*, from a combination of the principle of virtual velocities with the principle of D'Alembert—and who have appreciated the simplicity and harmony which he introduced into the research of the planetary perturbations, by the idea of the variation of parameters, and

[4] A detailed account of Hamilton's derivation of the analogy can be found in Hankins' biography of Hamilton (Hankins, 1980), which also treats the impact of the analogy on later physics and especially the development of wave mechanics.

[5] "Whether we adopt the Newtonian or the Huygenian, or any other physical theory, for the explanation of the laws that regulate the lines of luminous or visual communication, we may regard these laws themselves, and the properties and relations of these linear paths of light, as an important separate study, and as constituting a separate science, called often *mathematical optics*."(Hamilton, 1833, p. 314)

> the differentials of the disturbing function, 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, 1833, p. 315)

As one of the chief merits of his method Hamilton saw the fact that the same formal theory applies to the geometry of light rays irrespectively of whether one considers light to consist of particles (obeying a principle of least action) or of waves (obeying Huyghens' envelope theory). While the consistency of ray optics with the emission theory of light is immediately plausible (light rays are simply the paths of the light particles), Hamilton showed that his theory of the characteristic function can also be understood from a wave theory of light:

> It remains [...] to illustrate the mathematical view of optics proposed in this and in former memoirs, by connecting it more closely with the undulatory theory of light. (Hamilton, 1837, p. 277)

On the wave theory, the fundamental physical entity are not the rays but the surfaces of constant value of the characteristic function: they define the wave fronts of the light wave. Hamilton showed how Huyghens' construction of successive wave fronts leads again to the Hamiltonian partial differential equation, thus demonstrating the validity of his approach also in a wave theory of light. This, however, is only approximately true: At about the same time, Augustin Jean Fresnel began to argue that certain phenomena which can be described by ray optics only with the help of cumbesome additional assumptions were explainable much more straightforwardly in terms of wave optics. This implies that ray optics is only a limiting case of wave optics and that the two theories are not generally equivalent.[6] Hamilton does not seem to comment on this issue and it is not clear to us whether he was aware of this limit to his "general method."

In the following decades, the wave theory of light quickly became universally accepted and Hamilton's geometrical optics faded into oblivion even though it was the most general formulation of geometrical optics. In 1895, Heinrich Bruns rederived independently important parts of Hamilton's optics in his theory of the eikonal (Bruns, 1895). He pointed out the close formal analogy between the eikonal in geometrical optics and the Hamiltonian action integral in mechanics without realizing that Hamilton had arrived at Hamiltonian mechanics through this analogy. A clear presentation of the Hamiltonian formulation of ray optics as the limiting case of a wave equation was given by Sommerfeld and Runge (1911, p. 290), who credit Peter Debye with the idea for the derivation.

Only with Einstein's seminal work of 1905 (Einstein, 1905) did the corpuscular theory of light reemerge, and only at about the time of the genesis of wave mechanics did the question of the nature of light—and now also of matter—again become as open as in the early 19th century. De Broglie pointed out that a variational principle can be used to formulate a theory of light that transcends the distinction between particle and wave. But also he seems to have been unaware of Hamilton's pioneering work and in his dissertation he only speaks about the analogy between Fermat's principle in optics and Maupertuis's principle in mechanics.

What does all this have to do with mechanics? In direct continuation of his work on optics, Hamilton announced in 1833 that Lagrangian mechanics itself could be formulated in a way that is mathematically equivalent to his theory of ray optics. Hamilton was able to show that

[6] For the history of the dispute about wave optics in the early 19th century see (Buchwald, 1989; Buchwald and Smith, 2001).

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

Figure 2: Hamilton's optical-mechanical analogy: The two different interpretations of Hamilton's characteristic function in optics and mechanics.

both optics and mechanics obey the same variational principle for the same type of characteristic function. In mechanics, Hamilton's characteristic function is a generalization of the integral that Maupertuis had called 'action' and that had to be minimized in the least action principle. Therefore, Fermat's principle of the shortest time and the mechanical principle of least action are just specific formulations of Hamilton's more general principle.[7] The only fundamental difference between wave and particle picture in this scheme lies in the interpretation of the integrand of the characteristic function: In the particle picture, it represents the particle momentum while in the wave picture, it represents the inverse of the phase velocity (see Fig. 2). In both cases, the action integral can be found by solving the Hamiltonian partial differential equation, which therefore offers a most general method of solving dynamical problems. This constitutes the optical-mechanical analogy.

The optical-mechanical analogy led Hamilton to his formulation of mechanics nowadays known as Hamiltonian Mechanics. The dynamics of a system can be entirely derived from the knowledge of a single characteristic function:

> 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

[7] Hamilton (1833, p. 317) credits Maupertuis for the general idea of such an universal action principle.

> V; which is analogous to my optical function, and represents the action of the system from one position to another. (...) The development of this view, including its extension to other analogous questions, appears to me to open in mechanics and astronomy an entirely new field of research. I shall only add, that the view was suggested by a general law of varying action in dynamics, which I had deduced from the known dynamical law of least or stationary action, by a process analogous to that general reasoning in optics which I have already endeavoured to illustrate. (Hamilton, 1833, p. 332)

The unifying potential of Hamiltonian Mechanics was acknowledged and fueled widely-held beliefs that all of science was eventually to be based on variational principles such as the principle of least action. However, it only had limited practical impact on 19th century physics.[8] Hamiltonian mechanics was extended by the mathematician Carl Gustav Jacob Jacobi and became in this form an important tool for celestial mechanics. The root of Hamiltonian mechanics in his optics, on the other hand, was mostly forgotten outside of Great Britain.

One of the few exceptions was Felix Klein who already had pointed to Hamilton's work in optics in 1891 (Klein, 1892). When, as mentioned above, Heinrich Bruns noticed the similarity between his theory of the eikonal and Hamiltonian mechanics, Klein (1901) pointed out that this similarity reflected the historical roots of Hamilton's theory. Klein's own lecture notes on the derivation of Jacobian theory from optical considerations were only available in manuscript at the Göttingen library (Hankins, 1980; Schrödinger, 1926c). One of the few people that took notice of them was Klein's assistant Arnold Sommerfeld who wrote the above-mentioned paper with Iris Runge and years later would point out the convoluted history of the optical-mechanical analogy to Erwin Schrödinger.

Another thread in the reception of Hamiltonian mechanics in the 19th century, which also would become important for Schrödinger's development, is the tradition of the geometrization of mechanics, starting with Jacobi's elimination of time from the action integral which rendered the problem purely geometrical. The further history is intimately connected with differential geometry of variously curved spaces as developed by Gauss and Riemann.[9] Already Gauss had shown that a statement analogous to Malus's theorem (of the existence of surfaces orthogonal to light rays) holds for geodesics in a curved space. Beginning with Liouville, Lipschitz, and Darboux, French mathematicians realized that Hamilton-Jacobi mechanics could generally be understood as a theory of geodesics in a higher-dimensional space with variable curvature given by the kinetic energy. This approach was one of the roots of Heinrich Hertz's analytical mechanics. However, Hertz went further and eliminated the concept of force altogether by introducing hidden masses and mechanical constraints (*Bindungen*) which connected the visible matter to these hidden masses. Therefore, any mechanical motion is seen as a free motion in the manifold defined by the mechanical constraints. In this regard, Hertzian mechanics can be seen as a precursor of General Relativity, which however does not follow Hertz's idea of giving up the concept of force altogether.

[8]For the history of the reception of the optical-mechanical analogy in the 19th and early 20th century, see (Hankins, 1980, Chapter 14)

[9]This story is treated in detail by Jesper Lützen's excellent book on Hertzian mechanics (Lützen, 2005).

3. Schrödinger's work on analytical mechanics

Schrödinger, in two unpublished manuscripts[10] titled *Hertz'sche Mechanik und Einstein'sche Gravitationstheorie* attempted to develop the Hertzian idea of a geometrization of mechanics in a hope to connect it to Einstein's general theory of relativity (Mehra and Rechenberg, 1987a,b). In the first chapter of the manuscript, Schrödinger gives a programmatic introduction in which he poses the problem to find an intuitive understanding of general relativity and proposes to search this understanding in the relationship between General Relativity and Hertzian mechanics. He writes:

> Given these manifest internal connections between Hertzian mechanics and Einstein's General Relativity, it is hard for me not to attribute a deeper meaning to the circumstance that *in both cases the "forces" make their entrance in the same mathematical garb, namely as the Riemann-Christoffel three-indices symbols of a quadratic form of the coordinate differentials.* [11]

However, the manuscript breaks off and it does not become clear where Schrödinger hoped to find the deeper connection between Hertzian mechanics and General Relativity.

In the same context Schrödinger wrote three notebooks entitled *Tensoranalytische Mechanik*[12] in which he explored the Hertzian formulation of mechanics. The notebooks contain various speculations about a representation of mechanics in differential geometric form. Schrödinger uses elements of Hertzian mechanics, Liouville's geometric representation of mechanics, and General Relativity, exploring various connections between these ideas, without coming to clear conclusions. One line of thought, for instance, is the attempt to explain the rest mass of matter as the kinetic energy of a hidden motion in additional dimensions. Just as in the manuscripts, however, the fundamental motivation for Schrödinger's explorations seems to be the search for a common root of general relativity and the noneuclidean representation of analytical mechanics, with the hope of a better physical understanding and possible extension of both.

Especially noteworthy is that the the first notebook shows that Schrödinger tried to understand quantum conditions as constraints (*Bindungen*) in the sense of Hertzian mechanics (see also Mehra and Rechenberg, 1987a, pp. 220–226). In the Hertzian picture, as mentioned before, forces between particles are derived from constraints in a higher-dimensional space. These constraints determine the noneuclidean configuration space of the particles in which the actual trajectories are geodesics. Thus, forces have been completely eliminated. Since quantum conditions can also be seen as constraints in phase space, it seems that Schrödinger's hope was that he could reformulate the old quantum theory in such a way that both forces and quantum conditions would be represented by constraints in a higher-dimensional space. This would have led to a unification of the concept of force and the concept of a quantum condition.

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[10] The two manuscripts really form two parts of a continuing whole. Manuscript AHQP 39-3-004 seems to predate manuscript AHQP 39-3-005 but was later marked as chapter two. Manuscript 39-3-005 comprises chapters 1 and 3. Manuscript 39-3-004 is entitled *Hertz'sche Mechanik und Einstein'sche Gravitationstheorie*, but that title is crossed out, presumably when Schrödinger assigned it as chapter two for the extended manuscript.

[11] Schrödinger, AHQP 39-3-005, emphasis in the original (underlined).

[12] AHQP 39-3-001, 39-3-002, 39-3-003. Mehra and Rechenberg (1987b, p. 529) assume that the two manuscripts (AHQP 39-3-004, 39-3-005) predate the three notebooks and that the notebooks are an "immediate continuation" of the manuscript. However, it is just as plausible to speculate that the manuscripts grew out of the more general considerations of the notebooks.

Figure 3: Part of a page from Schrödinger's third notebook on tensor-analytical mechanics (39-3-003).

In the second notebook, Schrödinger starts by analyzing the concept of curvature in a Riemannian space. In this context,[13] he quotes (Weyl, 1918) and remarks:

> What we need for the principle of the straightest path is the concept of *parallel displacement of a vector belonging to a given point by an infinitesimal distance* and further by an integral distance, to say it more clearly, along a finite arc. The geodesic line as the *straightest* results through *continued parallel displacement of a line element in its (respective) direction! This is fundamental.*[14]

Schrödinger continues with an attempt to represent general forces through the curvature of a Riemannian space and asks himself how the metric tensor has to be defined to this end. Schrödinger's hope is that he can calculate the metric as a function of a scalar potential V and a total energy E so that the actual trajectories follow from a principle of least constraint. He realizes that he cannot directly calculate the metric since it depends on the motion itself. Rather he needs to calculate the action integral from the Hamiltonian partial differential equation, which, in this context, appears as a generalization of the Hertzian metric for the case of systems moving under the influence of external forces. Schrödinger writes:

> The metric tensor for the (q, t)-space can *not* be given for the general case. It depends on the motion itself. One has to solve the Hamiltonian partial differential equation first, in a certain sense as a field equation, one has to pick a suitable solution—and only *then* can one say: The trajectory of the system is an extremum of this field.[15]

Especially noteworthy in the light of what was to come is the idea expressed here that the Hamiltonian partial differential equation can be interpreted as a field equation. Thus the solution to the optical problem determines an "action field" that in turn determines—through an extremum principle—the trajectories that solve the mechanical problem. This means that the "field" given by the wave fronts is ontologically prior to the trajectories whose shape is determined by this field.

These considerations lead Schrödinger to a more extensive inquiry into the geometric interpretation of the Hamiltonian partial differential equation and, especially, Hamilton's optical-mechanical analogy in the third notebook (AHQP 39-3-003). The second part of the notebook is entitled "Analogies to Optics. Huyghens' principle and Hamiltonian Partial Differential Equation" (see Fig. 3). After juxtaposing the mechanical principle of least action and the optical principle of least time, Schrödinger explores how Huyghens' principle is used to construct surfaces of equal time in an optical medium and how rays are constructed as orthogonals of such surfaces of equal time. This also implies that these rays fulfill an extremum principle, the principle of shortest time. After some further explorations of geometrical optics follows a section entitled "Direct transfer to mechanics." Here, Schrödinger applies the construction to the case of mechanics by replacing the time integral along the optical ray with the action integral along

[13] This gives a lower bound for the dating of this section of the notebook AHQP 39-3-002.

[14] Schrödinger, AHQP 39-3-002, emphasis in the original (underlined).

[15] *ibid.*, emphasis in the original (underlined).

the trajectory and obtains the Hamiltonian partial differential equation and the Lagrangian equations of motion. Except for the fact that Schrödinger expresses the kinetic energy as a covariant metric over the velocities, this section does not show any attempts at an extension of classical mechanics. It does show, however, Schrödinger's acquaintance with and constructive application of Hamilton's optical-mechanical analogy as early as 1918–1922.

The study of Schrödinger's attempts to generalize mechanics sheds new light on the "Remarkable Property" paper (Schrödinger, 1922). Here, as in the remark on Weyl in the notebooks quoted above, Schrödinger is concerned with the parallel displacement of a vector in curved space, and as in the notebooks he is looking for a physical justification for quantum conditions. Although the notebooks don't show any awareness of Weyl's gauge theory, the similarity of intentions and outlook is obvious. Therefore, the "Remarkable Property" paper can be seen as an offspring of Schrödinger's much more general program of extending mechanics and not just, as Raman and Forman (1969) see it, as a singular piece of evidence for Schrödinger's developing interest in atomic physics in the early 1920s. As we will argue in the next section, it is this more general program that later would trigger Schrödinger's interest in de Broglie and that eventually would be transformed into his research program in wave mechanics.

4. The genesis of wave mechanics: Hamilton's analogy as a heuristic tool

When de Broglie proposed the idea of matter waves, he explicitly used the analogy between ray optics and classical mechanics to justify his proposal.[16] However, he seems unaware of Hamilton's formulation of the optical-mechanical analogy. De Broglie represented the analogy as the formal equivalence of Fermat's principle of the shortest path and Maupertuis's principle of least action. It is remarkable that de Broglie had already arrived, from relativistic considerations, at the conclusion that the phase velocity of the matter wave is inversely proportional to the velocity of the corresponding particle, which exactly matches the relation in the optical-mechanical analogy (see Fig. 2).

Schrödinger learned from Einstein about de Broglie's idea in the context of gas statistics.[17] Schrödinger's interest in this subject grew out of his devotion to a Boltzmannian program of statistical mechanics. In 1924, Schrödinger investigated Planck's derivation of the Sackur-Tetrode quantum theory of the ideal gas which had been criticized by various authors, foremost Paul Ehrenfest, as being *ad hoc*. The essential point of Ehrenfest's criticsm was Planck's division of the state function by a factor $N!$ in order to make entropy an extensive quantity. Planck justified this division with the observation that, without this division, permutations of identical particles would be counted separately. Ehrenfest countered that Planck's counting procedure was mathematically incorrect and that entropy need not be an extensive quantity in any case. Schrödinger was already involved in this discussion when Einstein published his paper "Quantentheorie des einatomigen idealen Gases" (Einstein, 1924) which used Bose statistics to derive a state function of the ideal gas. Einstein had derived the density fluctuations of a Bose-Einstein gas and shown that they showed the same duality of a "wave term" and a "particle term" as the density fluctuations of blackbody radiation. He quoted de Broglie's dissertation as a promising approach to understand this mysterious duality.

[16]For a historical account of de Broglie's theory see e.g. (Jammer, 1966; Kubli, 1970; Darrigol, 1986).

[17]For Schrödinger's work on gas statistics and its role for the development of wave mechanics, see especially (Hanle, 1975, 1977).

Schrödinger argued that the Bose-Einstein statistics is a mathematically correct way of taking into account the identity of particles but he was unsatisfied with the fact that the counting of cases seemed physically unnatural:[18]

> For the time being, we are lacking any means to understand the strange kind of interaction between the moclecules which is supposed to lead to the cancellation of the number of permutations [i.e., what is called today indistinguishability] from the statistical calculus. The gas molecules would have to be something completely different, as Planck and Einstein have stressed themselves, and they must act onto each other completely differently than we had imagined so far. (Schrödinger, 1925)

Reading de Broglie's thesis in the fall of 1925, Schrödinger realized the connection of de Broglie's work to his his earlier attempts to make sense of the quantum conditions and to his paper of 1922.[19] However, much more fundamental than this formal similarity is that de Broglie's explicit use of the optical-mechanical analogy as a heuristic argument for the wave representation of matter must have resonated strongly with Schrödinger. As we have seen, he had pondered the optical-mechanical analogy with a similar motivation of extending classical mechanics himself. But as we will show, the role of the optical-mechanical analogy was not limited to making Schrödinger receptive to de Broglie's ideas, it also played an important role in his development of these ideas.

First however, de Broglie's idea of matter waves helped Schrödinger to see light in the quantum theory of the ideal gas: On December 15, 1925, he submitted his paper "On Einstein's Gas Theory." In this paper, Schrödinger wrote:

> A natural feeling rightfully objects against considering this new [Bose-Einstein] statistics as something primary, not amenable to further explanation. (Schrödinger, 1926a, p. 95)

Schrödinger argued that matter waves offer a natural way to give a physical understanding to the otherwise mysterious Bose counting procedure that Einstein had applied to the ideal gas. Understanding particles as wave modes explains the indistinguishability of particles that is characteristic for the Bose-Einstein statistics. Unlike his contemporaries who were willing to accept the existence of a statistics *sui generis* for microscopic particles, Schrödinger saw the fact that the wave picture would lead back to a classical Boltzmann statistics as a strong indication for the correctness of the wave picture of matter. Therefore, the success of Einstein's gas theory was for him a strong argument to "get 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." (Schrödinger, 1926a, p. 95)

This indicates that also this root of wave mechanics can be seen in the context of Schrödinger's general program of extending mechanics. We only need to take note of the interpretation of statistics expressed in the quote from "On Einstein's Gas Theory" above. Schrödinger's search for a "natural statistics" reflected his realistic approach to statistical mechanics strongly influenced by Boltzmann's work: It is not merely a phenomenological theory, which can be formulated quite

[18] See (Howard, 1990) for the debate about the statistical correlations in Bose-Einstein statistics.

[19] Schrödinger remarked on this connection in his letter to Albert Einstein dated November 3, 1925 (see Moore, 1989, pp. 191–192). The letter dates Schrödinger's reading of de Broglie quite precisely: He states that he read the dissertation "a few days ago."

independently of the nature of the underlying mechanism. Rather, statistical behavior reveals the true structure of the building blocks of the physical world.[20] Given this realistic approach to statistics, Schrödinger's work in gas statistics is tied quite closely to his foundational interests in mechanics.

Schrödinger quickly "got serious" about de Broglie's idea and, probably during his Christmas vacation in 1925, tried to formulate a wave equation to give an exact description of de Broglie's matter waves.[21] He quickly realized that this wave equation made good on the program already stated in his notebooks on tensor-analytical mechanics: it offers a physical explanation for quantization rules. The discrete quantum levels can now be explained as the discrete solutions resulting from the eigenvalue problem of the wave equation, just as a vibrating body can only oscillate in specific discrete modes. Equally, the discrete orbits of the Bohr atom can be understood as discrete wave modes of the electron waves.

A later reminiscence attributes the idea to derive a wave equation to a remark made by Debye when Schrödinger presented de Broglie's dissertation in a Zürich colloquium (Bloch, 1976). Such a hint, however, seems unnecessary given Schrödinger's firm acquaintance with classical wave theory evident from the lecture notes he took as a student in Vienna (AHQP, Film 39). Schrödinger himself prominently used the optical-mechanical analogy as a heuristic argument for the derivation of a wave equation for matter in his second communication on wave mechanics (Schrödinger, 1926c). Does this imply that it was the Hamiltonian analogy that led him to the wave equation? Then, however, it is striking that the first communication (Schrödinger, 1926b) does not mention the optical-mechanical analogy and derives the wave equation rather *ad hoc* from an abstract variational principle. This led to the assumption that Schrödinger might not even have known about the analogy at the time he wrote his first communication.[22] As discussed above and first pointed out by Raman and Forman (1969), Schrödinger was certainly well aware of the analogy since the late 1910s. This makes the omission of a reference to the optical-mechanical analogy in the first communication quite surprising. An extended discussion has arisen in the literature whether the optical-mechanical analogy played a role in the discovery of the wave equation or whether the succession of the communications reflects the the fact that Schrödinger discovered the wave equation independently from the Hamiltonian analogy. Even without using the evidence from the earlier notebooks, Wessels (1979) doubts that the analogy played no role in Schrödinger's thinking and distinguishes a heuristic role that the Hamiltonian analogy played for the discovery of the wave equation from the constructive role it played in the second communication.

Kragh (1982) uses the evidence from the early notebooks to argue for the importance of the analogy in Schrödinger's thinking and points out that Schrödinger mentions the "Old Hamiltonian analogy" already in the notebook written for the first communication (AHQP 40-5-003) even though it doesn't appear in the published text. On the other hand, he also recognizes that the earliest preserved notes on wave mechanics by Schrödinger (AHQP 40-5-002) do not arrive at the wave equation from the Hamiltonian analogy. It is of course not certain that these notes,

[20] See (Wessels, 1983) for a discussion of the relationship between Schrödinger's methodology in statistics and his search for intuitive pictures of physical reality.

[21] There is some debate in the literature about the exact date of Schrödinger's first attempt, which is recapitulated in (Kragh, 1982), but as Kragh shows, the possible time frame is rather short, between Schrödinger's letter to Einstein from November 3 (see above) and Schrödinger's letter to Wien on December 27, see below. In any case, the precise dating of this attempt is not essential to our argument, but only that it can be identified with the notes AHQP 40-5-002 as we argue below.

[22] Letter from Erwin Fues to Thomas S. Kuhn, Oct. 31, 1963, quoted in (Wessels, 1979).

entitled “H-Atom. Eigenschwingungen”, really represent Schrödinger’s first attempt to derive a wave equation. However, we do think that it is highly plausible for internal reasons: Schrödinger writes in a letter to Arnold Sommerfeld from Jan. 29, 1926, (Sommerfeld, 2004, pp. 236-238) that he recognized the coefficients from Sommerfeld’s solution of the Hamiltonian partial differential equation for the relativistic Kepler problem in his own early calculations and that this gave him confidence that he was on the right track. AHQP 40-5-002 contains Sommerfeld’s coefficients, and therefore it is plausible that these are the calculations that Schrödinger refers to in the letter. Also Mehra and Rechenberg (1987b) study these notes in detail and come to the conclusion that they constitute Schrödinger’s first attempt at deriving a wave equation. They show that Schrödinger, without actually solving the relativistic wave equation he had found, was able to see that it would lead to noninteger quantum numbers different from Sommerfeld’s result. [23] That was the reason that Schrödinger himself gave why he abandoned his first attempt at a relativistic wave equation. These reasons make it seem very probable that AHQP 40-5-002 really was Schrödinger’s first attempt at a wave equation. But in these notes, Schrödinger makes no reference to the Hamiltonian analogy or a variational principle: he obtains the wave equation simply from inserting the known velocity of the de Broglie phase wave into a generic relativistic wave equation. Thus, the Hamiltonian analogy was not the way through which Schrödinger arrived at the wave equation originally, he rather used a very simple and straightforward abduction from de Broglie’s determination of the matter wave velocity.

Nevertheless, Schrödinger turned to the optical-mechanical soon after, he mentions it in AHQP 40-5-003, which was certainly written before the first communication, as Kragh (1982) points out. An even more substantial point about the role of the Hamiltonian analogy can be made from a thorough study of this notebook: We will argue that the abstract variational principle presented in the first communication was found by Schrödinger through his occupation with the Hamiltonian analogy. The seemingly *ad hoc* variational principle is a stand-in for a more complex thought process motivated by the optical-mechanical analogy. AHQP 40-5-003 begins with the treatment of the nonrelativistic case, or more exactly with an approximation for particle velocities small compared to the velocity of light. Therefore it is plausible to assume that this notebook was written in direct continuation of the failed relativistic derivation of AHQP 40-5-002, trying out what would happen if relativity was not taken into account. Schrödinger mentioned results from this section of the notebook in a letter to Wilhelm Wien dated Dec. 27, 1925 which implies that he must have started the notebook by that time. Among various rather preliminary calculations for the Stark and Zeeman effects, Schrödinger spends a considerable effort on finding a variational principle that would yield the wave equation just as a variational principle in elasticity theory yields the corresponding wave equation. After several unsuccessful attempts at guessing the variational principle, there appears in the notebook a program that contains as its second item “the old Hamiltonian analogy between optics and mechanics”. In the text corresponding to this item, Schrödinger starts from the Hamiltonian partial differential equation and reinterprets it as a variational principle which indeed leads him to the (nonrelativistic) wave equation. This exactly mirrors the beginning of Schrödinger’s first communication that mystified later commentators. The context of the notebook entry shows that the invocation

[23] Sommerfeld’s theory seemed at the time well confirmed by the empirical facts, since it explained the obseved fine structure of hydrogen. That agreement turned out to be coincidental since Sommerfeld, just like Schrödinger, had not taken into account electron spin. Sommerfeld’s theory, however, also used a classical expression for total angular momentum, instead of the quantum mechanical value. This just canceled the error from the neglect of spin (Granovskii, 2004), while in Schrödinger’s case the problem became visible.

of the variational principle is not an alternative to an argument from the Hamiltonian analogy but, quite to the contrary, is motivated by the analogy. This connection between the variational principle and the Hamiltonian analogy gets clearer if we consider Schrödinger's previous work on tensor-analytical mechanics.

As we pointed out above, Schrödinger had already thought about a "field" interpretation of the Hamiltonian partial differential equation in his second notebook on tensor-analytical mechanics. He now tried to think of de Broglie's waves as defined by a suitable generalization of the Hamiltonian partial differential equation. Already around 1918, Schrödinger had interpreted the Hamiltonian partial differential equation as defining an "action field" that specifies a variational principle for the matter trajectories. He now transposed the two steps of solving the field equation and solving the variational problem to obtain a variational principle for the wave equation. This is the only difference to his earlier procedure from 1918. Of course, the permutation of the two steps *is* in fact quite *ad hoc*:[24] The variational principle does not follow in any strict sense from the Hamiltonian analogy and Schrödinger's use of the analogy is purely heuristic. Rather, its use shows the interplay between heuristic ideas and formal analogies characteristic for the creation of new theories out of the elements of existing knowledge, which was discussed for the case of Einstein's development of the theory of general relativity in (Renn and Sauer, 2007). Schrödinger's notebooks resolve the mystery of the seemingly *ad hoc* introduction of the variational principle in Schrödinger's first communication and show that behind it stands Schrödinger's continuing exploration of the optical-mechanical analogy.

5. The search for a relativistic wave equation: Hamilton's analogy as a formal constraint

Already in the introduction to his second communication on wave mechanics (submitted less than a month after the first), titled "The Hamiltonian analogy between mechanics and optics," Schrödinger discards his initial derivation of the wave equation as being unintelligible:

> For the time being, we had described this connection [between the wave equation and Hamilton's partial differential equation] only briefly in terms of its outward analytical structure by means of the *per se* unintelligible transformation (2) [defining the wave function as the logarithm of the classical action] and by means of the likewise unintelligible transition from setting an expression to zero to the requirement that the space integral of that expression be stationary. (Schrödinger, 1926c, p. 489)

He then moves on to present a new derivation that draws heavily on the Hamiltonian analogy. What made Schrödinger return to the optical-mechanical analogy? We argue in this section that the new derivation of the wave equation in his second communicaton arose in the context of Schrödinger's unsuccessful attempts to derive a relativistic wave equation that would replace the nonrelativistic one presented in the first communication. Schrödinger hoped that the relativistic equation would allow him to take into account in a natural way the interaction of the wave function and the electromagnetic field. In that case, he would be able to explain the Zeeman effect and calculate the coefficients of emission and aborption of electromagnetic radiation within the wave-mechanical picture, thus going well beyond the old quantum theory and the rival matrix

[24] Nevertheless, the connection between the classical variational principle and Schrödinger's variational principle for the wave function can be clarified formally. It can be shown that the classical principle is a limiting case to Schrödinger's. See (Gray, Karl, and Novikov, 1999).

mechanics. Moreover, we want to show that the new derivation involved a fundamental change in the role of the optical-mechanical analogy in Schrödinger's reasoning.

The crucial progress for Schrödinger was the completion of Hamilton's optical-mechanical analogy: Hamilton's analogy consists of a formal relationship between corpuscular mechanics and ray, not wave, optics. Thus, the wave equation for matter cannot be the formal analog of Hamilton's partial differential equation. Rather, it has to transcend Hamilton's partial differential equation in the same way as wave optics transcends ray optics, the latter being merely a limiting case of the former. Schrödinger is very explicit on this point in his second communication:

> 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 an "undulatory mechanics"—and the obvious way to this end is the wave-theoretical extension of Hamilton's picture. (Schrödinger, 1926c, pp. 25)

Until the present study of his notebooks, it has remained unclear whether Schrödinger possessed this knowledge already when he first derived a wave equation. We will demonstrate below that this insight only occurred to him after the completion of his first communication.

The first notebook in which Schrödinger explicitly utilized the results of his first communication is titled "Eigenwertproblem des Atoms. II" (AHQP 40-6-001). It begins with a section titled "Für die II. Mitteilung" which lays out the Hamiltonian analogy. Interestingly, Schrödinger's notes do not correspond at all to the later content of his second communication. Schrödinger first sets out to "clear up the rather obscure relationship between Hamilton's partial differential equation (1)[25] and the wave equation (5)": He claims that the Schrödinger equation[26] (5) simply is the wave equation that gives, when solved, the wave fronts satisfying Hamilton's partial differential equation (or at least is one possible such wave equation). This is, however, only approximately true, as Schrödinger would state very cleary in the quote from the second communication above. The interesting observation is that in the notebook Schrödinger does not yet realize this decisive restriction: He searches for a wave equation that will be exactly equivalent (and not just in the appropriate 'ray optical' limit) to the Hamiltonian partial differential equation. Citing Whittaker,[27] Schrödinger recapitulates Hamilton's formal analogy between mechanics and optics and Hamilton's construction of the surfaces of constant action through Huyghens' principle. He states again, even more explicitly, that it is *obvious* that the Schrödinger equation will give the desired surfaces of constant action, confirming our previous observation.

Schrödinger next considers the form of Hamilton's partial differential equation that contains time explicitly. He observes that it is nonsymmetrical in time and space coordinates. Therefore, he turns to the relativistic version of Hamilton's partial differential equation, introducing canoncial momenta and the four-potential. He observes that now, instead of the gradient of the action, the four-gradient of the action minus the four-potential enters the geometrical construction of wavefronts in four-dimensional space and tries to gain an intuitive understanding of this fact by

[25]The notebook contains references to the equations of the first communication using the exact same numbers as used in the published manuscript. In addition, a note added in proof to the first communication can be found *verbatim* in this notebook.

[26]For the sake of brevity, we will attach this slightly ahistorical label to the nonrelativistic wave equation for the matter wave that Schrödinger had postulated in the first communication.

[27]Presumably (Whittaker, 1904), the German edition of which Schrödinger refers to in the second communication.

comparing it to a wave in a medium with a flow. Schrödinger tries to construct the wavefronts in the relativistic case, again through an application of Huyghens' principle. He is not able to show that this leads to the Hamiltonian partial differential equation and breaks off. Instead he tries to directly solve the wave equation in a flowing medium, hoping that "maybe the correction will come out by itself." However, the resulting wave equation is too complicated, and again he cannot show that it leads to Hamilton's partial differential equation. Next follows a reconsideration of the extremum principle of the first communication under the heading "Connection between the wave equation and the Hamiltonian equation." Again, Schrödinger uses the equation $S = K \log \psi$ as an exact equality and tries to show with its help the equivalence of the Hamiltonian partial differential equation and the variational principle. The attempt breaks off with the remark "I'm not moving ahead!" After another attempt at direct construction of the wave equation (this time through an odd non-Lorentzian transformation of the wave equation), he gives up his foundational explorations and uses the rest of the notebook for studying perturbation theory and the Stark effect. The remarkable feature of all these attempts to find a relativistic wave equation is that they are based on an exact functional dependence of the Hamiltonian action S and the wave function ψ.

Also AHQP 40-7-001, titled "Eigenwertproblem des Atoms. III," is a notebook written by Schrödinger before the second communication on wave mechanics. Hence, it appears to be the direct continuation of AHQP 40-6-001. It is in this notebook, again in a section titled "for the second communication," that Schrödinger takes a crucial step forward that leads him to the completion of Hamilton's optical-mechanical analogy. He writes:

> For the second communication:
>
> Naturally, one must not expect that any explicit function of S itself satisfies the wave equation (for instance $\cos S$, or the like). For S is only the phase of the wave, say, the time at which a certain wave front reaches the point P in configuration space, expressed as a function of the coordinates of P. Thus, $\cos S$ is only the wavefunction disregarding the amplitude. The latter naturally also has to be assumed to vary as soon as the rays diverge or converge if a wave equation is to hold. And since this diverging and converging of the wave normal is not equal in all points of a wavefront, the amplitude does not vary along all rays in a proportional way. Therefore, one cannot give a general function of S alone that satisfies the wave equation.
>
> The transition from Hamilton's partial differential equation to the wave equation thus signifies in mechanics the exact same thing as in optics the transition from ray optics, which is generated merely by Fermat's principle, to wave optics proper. One can speak of an undulatory theory of mechanics. Symptomatically, one encounters exactly the same indeterminacy as back then in optics: Initially, one only knows the speed of propagation and does not know how this speed is to be assigned to a specific elasticity and density [of the medium] respectively. (AHQP 40-7-001)

What had escaped Schrödinger so far was the full impact of the fact that the connection established by Hamilton between wave optics and ray optics does not entail a complete equivalence of the two optical theories, but that ray optics is only a limiting case of wave optics. Schrödinger had not understood what this meant for the relationship of classical and wave mechanics at the time he wrote his first communication: He did not realize that wave mechanics does not just impose additional constraints on classical motions (i.e. that it leads to quantum conditions), but that it means that the motions predicted by classical mechanics are only an approximation to the evolution of a full wave field. When Schrödinger tried to construct the wavefronts in the relativistic case, he failed in AHQP 40-6-001 because he was misled into believing that the full wave function would result from the relation $S = k \log \psi$. That decisive insight, possibly due to the correspondence with Sommerfeld,[28] is reflected in AHQP 40-7-001, quoted above: Here Schrödinger realized that S would only give him the phase of a more general wavefunction and that he needed to go beyond the picture of wave fronts determined by the classical action in order to also recover the amplitude of ψ. Schrödinger (1926c, p. 489, footnote 2) explicitly states his error in a footnote to the introduction of his second communication.

Thus, AHQP 40-7-001 contains Schrödinger's decisive new idea: Wave mechanics is a more general theory than particle mechanics in the same sense as wave optics is more general than geometrical optics. Hamilton's analogy is only one axis in a four-way correspondence (see Fig. 4). It establishes a connection between classical mechanics and ray optics, but fails to establish a direct connection between classical mechanics and the more general wave mechanics. Rather, the direct connection is between wave optics and wave mechanics. But this has a direct impact on the interpretation of the analogy: what the analogy means is that matter *really* consists of waves, just as Fresnel had found that light *really* consists of waves. The "old" Hamiltonian analogy, by its completion, changed its role from a heuristic tool (as employed in the course of writing his first communication) to a formal constraint: wave mechanics has to reduce to classical mechanics in the limit of wavelengths that are short compared to the curvature of the classical trajectories. This is an extension and justification of Bohr's correspondence principle, and Schrödinger hoped to use this constraint for the construction of a new mechanics—wave mechanics—that would be more general and powerful than both the Bohr-Sommerfeld quantum theory and the Göttingen matrix mechanics. Through the analysis of the notebooks, it is clear that this insight occurred to Schrödinger only after his completion of the first communication and that it resulted from his unsuccessful attempts at generalizing the non-relativistic wave equation for the atom.

As we can see from the notebooks, Schrödinger had originally intended to present a full-fledged relativistic theory in his second communication. This is obvious from his early drafts for the second communication in AHQP 40-6-001 and only natural, given the fact that Schrödinger's point of departure was de Broglie's relativistic treatment of matter waves. However, also the new understanding did not lead to a different relativistic wave equation, and Schrödinger's attempts to find a complete theory of the coupling of the wave function and the electromagnetic field got bogged down in further complications that we will discuss in the next section. Therefore, the whole project was not even mentioned, and Schrödinger limited himself to treat further successful applications of the non-relativistic equation. Nonetheless, the new view of the the optical-mechanical analogy was also useful as an intuitive justification and physical interpretation of wave mechanics. This is how Schrödinger presented it prominently in the second communication.

[28] In the second communication, Schrödinger thanks Sommerfeld for pointing out Felix Klein's discussion of the optical-mechanical analogy (Klein, 1892, 1901) to him. He also quotes (Sommerfeld and Runge, 1911), which treats the relation of wave optics and Hamiltonian optics in a most perspicuous way. If Schrödinger had known this work earlier, it would be hard to imagine why he should have tried to derive the wave function by the direct *Ansatz* $S = k \log \psi$ in his earlier attempts. It seems quite plausible that Sommerfeld would have also pointed out this latter work to Schrödinger. Unfortunately, several letters from Sommerfeld to Schrödinger in the spring of 1926 are lost whose existence we can infer from Schrödinger's answers. (See (Sommerfeld, 2004) for the existing correspondence.)

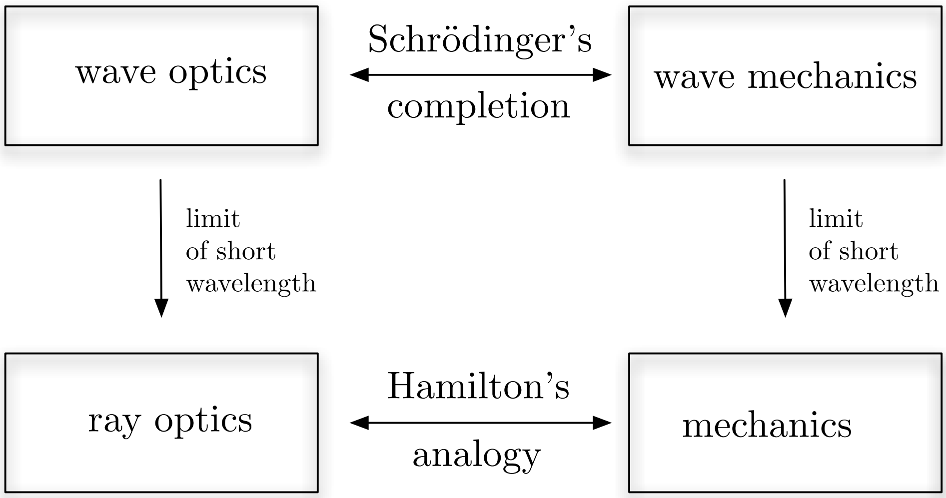

Figure 4: Schrödinger's completion of the Hamiltonian analogy between optics and mechanics.

6. The "pending questions": Hamilton's analogy as an interpretational device

In the following months, Schrödinger kept publishing at a rapid speed, continuing his presentation of nonrelativistic wave mechanics with two more communications that demonstrate the predictive power of the nonrelativistic wave equation, e.g. through the perturbative results for the Stark effect (Schrödinger, 1926e,f), and connecting it to matrix mechanics with the paper "On the Relation of the Heisenberg-Born-Jordan Quantum Mechanics to Mine" (Schrödinger, 1926d), giving the first published account of a formal connection between matrix and wave mechanics.[29] However, Schrödinger was also fully aware of the limitations of what he had achieved so far: not only did he not yet have a relativistic wave equation or a systematic account of electromagnetic interaction, an even more basic question still had to be answered: The wave function was not defined in 3-dimensional space, as one should expect if one was to think of it as any kind of physical wave. Rather it was defined in *configuration* space, which has $3N$ dimensions if N is the number of involved particles. There is no straightforward relation between a function on $3N$ dimensions and one on three dimensions, or even N different functions on three dimensions.[30] To recover a classical picture, Schrödinger therefore had to search for some three-dimensional functional of the full wave function representing the physical effects of the wave function (for example, representing the charge-current density as the source of the electromagnetic field). Hence, the problem of finding a physical interpretation of the wave function was intimately connected

[29] Also for this paper a preparatory notebook is preserved, AHQP 41-2-001, tentatively dated in AHQP to 1927, but clearly written before the publication of (Schrödinger, 1926d).

[30] Schrödinger notes this problem in a letter to Arnold Sommerfeld (February 20, 1926), mentions it in (Schrödinger, 1926c, p. 526) and discusses it more extensively in (Schrödinger, 1926f, p. 135). The problem also is noted by Hendrik Antoon Lorentz (letter to Schrödinger from May 27, 1926)

Figure 5: Attempt at an interpretation of $\psi \partial_t \psi$ as a density (AHQP 41-4-001).

with the previously mentioned problem of the coupling of matter wave and electromagnetic field, and so also with the question of the relativistic wave equation.

In the spring of 1926, the private and public research programs thus began to diverge. While focusing on successful applications of the nonrelativistic wave equation in his published work, Schrödinger's notebooks show him working intensively on the "pending questions"[31] of his more general program, which he only rarely alluded to in his published work. Especially noteworthy for this is the notebook entitled "Coupling. Very Old" (AHQP 41-4-001), in which he explores various expressions for the charge-current-density connected with the wave function (see Fig. 5). Therefore, it is most probably from the time before he settled on $\bar{\psi}\psi$ as the expression for the charge density, which he discussed in (Schrödinger, 1926f, p. 134-139). (This latter expression is explored in the presumably following notebook, AHQP 41-4-002.) In this notebook, an interesting tension in Schrödinger's research strategy can be observed: At various points, he still starts with the classical Hamiltonian partial differential equation and tries to generalize it to a wave equation. But mostly he tries to tackle the problem more directly, presumably in an attempt to find an alternative to the relativistic wave equation he still believes he has to abandon. These are the places where he tries various expressions for a charge-current density derived from the wave function and uses those to derive a wave equation with a coupling term to the electromagnetic field. This amounts to abandoning the idea of finding the wave function through a generalization of the classical Hamiltonian approach, where the "action field" is an abstract entity that cannot carry a physical charge, but obviously the physical plausibility of the step won out over such formal considerations, if Schrödinger even entertained them. Because that was what he believed he had learned from his struggle with the optical-mechanical analogy: the failure of classical mechanics means that matter *really* consists of waves, just like the failure of ray optics meant that light *really* consisted of waves. Ironically, the success of the optical-mechanical analogy now induced Schrödinger to abandon its use as a constructive tool and replace it with the use as an interpretational device.

This commitment became decisive when, in the summer of 1926, Max Born proposed the probabilistic interpretation of the wave function. Schrödinger objected vehemently—not surprisingly, since for him this meant a return to the obsolete particle picture and its quantum jumps. In opposition to the mainstream, Schrödinger insisted on a field interpretation of the wave function, guided by his literal reading of the optical-mechanical analogy. This is not the place to follow the ensuing debate between Schrödinger on one side and Bohr and the Göttingen school on the other. But the story told here should help to understand Schrödinger's deep commitment to the field interpretation for the rest of his life, which persisted even after he stopped opposing the probabilistic interpretation publicly after the Solvay meeting of 1927. Schrödinger was never satisfied with the Copenhagen orthodoxy, and would eventually resume his critique in the thirties and turn to unified field theory in a search for answers to the "pending questions."

[31] This is the title of the notebook AHQP 41-2-002.

7. Conclusion

The optical-mechanical analogy played a central role in Schrödinger's reception and development of wave mechanics. He first explored the analogy in the context of an ambitious program of generalizing classical mechanics around the end of World War I. When Schrödinger encountered the analogy again in de Broglie's dissertation, it attracted his attention and became a preliminary heuristic model for the development of his ideas. His struggle for a deeper understanding of the analogy in the search to overcome the limitations of the nonrelativistic wave equation led to the account in the second communication. We argue that only at this point he understood the full impact of his wave equation: classical mechanics is only an approximation to the 'undulatory mechanics' he was proposing. The optical-mechanical analogy became a formal constraint for his continuing search for a relativistic wave equation, and at the same time an intuitive justification for his programm. The success in the struggle for a reinterpretation of the optical-mechanical analogy reinforced his commitment to a physical wave interpretation of the quantum mechanical state and led to the first interpretation debate in quantum mechanics.

The changes in Schrödinger's use of the optical-mechanical analogy, already noticed by Wessels (1979), can be traced in Schrödinger's research notebooks, which offer a much more complete picture of the development of wave mechanics than has been generally assumed (e. g. (Moore, 1989)). The notebooks document every step in the development and give us a more extensive and more coherent picture of Schrödinger's thinking and aspirations than what was previously thought possible on the basis of the available evidence.

There is a striking similarity in the development of Schrödinger's use of the Hamiltonian analogy to the complex history of Einstein's use of the principle of equivalence in the development of General Relativity (See M. Janssen, 'No success like failure...': Einstein's quest for general relativity, 1907–1920. In M. Janssen and C. Lehner (Eds.), *The Cambridge Companion to Einstein*, forthcoming). In both cases, the emerging picture serves as a corrective to an overly simplistic reading of Thomas Kuhn's concept of incommensurability. Even in fundamental revolutions of the scientific world picture, it is insufficient to describe the theoretical development as a wholesale replacement of one conceptual system through another. Rather, the historian (and also the philosopher) needs to pay close attention to the often quite intricate process of transformation and reinterpretation of previously accepted knowledge.

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