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How Sommerfeld extended Bohr's model of the atom (1913–1916)

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Abstract. Sommerfeld's extension of Bohr's atomic model was motivated by the quest for a theory of the Zeeman and Stark effects. The crucial idea was that a spectral line is made up of coinciding frequencies which are decomposed in an applied field. In October 1914 Johannes Stark had published the results of his experimental investigation on the splitting of spectral lines in hydrogen (Balmer lines) in electric fields, which showed that the frequency of each Balmer line becomes decomposed into a multiplet of frequencies. The number of lines in such a decomposition grows with the index of the line in the Balmer series. Sommerfeld concluded from this observation that the quantization in Bohr's model had to be altered in order to allow for such decompositions. He outlined this idea in a lecture in winter 1914/15, but did not publish it. The First World War further delayed its elaboration. When Bohr published new results in autumn 1915, Sommerfeld finally developed his theory in a provisional form in two memoirs which he presented in December 1915 and January 1916 to the Bavarian Academy of Science. In July 1916 he published the refined version in the *Annalen der Physik*. The focus here is on the preliminary Academy memoirs whose rudimentary form is better suited for a historical approach to Sommerfeld's atomic theory than the finished *Annalen*-paper. This introductory essay reconstructs the historical context (mainly based on Sommerfeld's correspondence). It will become clear that the extension of Bohr's model did not emerge in a singular stroke of genius but resulted from an evolving process.

Introduction

Niels Bohr's atomic model was published in July 1913 in the first part of a "trilogy" of papers in the *Philosophical Magazine* [Bohr 1913]. Its historical origins have been described in great detail [Aaserud and Heilbron 2013; Heilbron and Kuhn 1969]. The related correspondence, manuscripts and publications have been subject of considerable editorial effort [Hoyer 1981].

The extension of Bohr's model to the Bohr-Sommerfeld model has also been scrutinized from various perspectives [Kragh 1985, 2012; Nisio 1973; Robotti 1986].

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Sommerfeld presented this extension first to the Bavarian Academy of Science in two memoirs in December 1915 [Sommerfeld 1915b] and January 1916 [Sommerfeld 1916a] (translated in English in this issue as [Sommerfeld 2014a] and [Sommerfeld 2014b]). They were omitted in Sommerfeld's Collected Works in favor of his subsequent publication in the *Annalen der Physik* [Sommerfeld 1916b]. An even more refined version is presented in Sommerfeld's legendary *Atombau und Spektrallinien*, first published in 1919, with almost annual new editions in 1920, 1922, 1923 and 1924, and its English translation *Atomic Structure and Spectral Lines* published in 1923 – to name only those editions that appeared before the advent of quantum mechanics in 1925 [Eckert 2013b]. From a historical vantage point, however, the Academy treatises deserve more interest because they reveal Sommerfeld's approach prior to their presentation "in refined form"[1] in the *Annalen* and in *Atombau*.

In this essay I will describe the context from which Sommerfeld's memoirs emerged[2]. The focus is on the time span between July 1913 and December 1915, which may be regarded as the gestation period, and the subsequent six months that Sommerfeld dedicated to their "refinement".

Sommerfeld's early reaction to the Bohr atom, 1913–1914

If Bohr's paper in the *Philosophical Magazine* with the pretentious title "On the Constitution of Atoms and Molecules" caused some interest it was more because of its content than its author. Bohr had finished his studies only two years earlier in Copenhagen and was hardly known among the international physicists. Sommerfeld's response to Bohr's atomic model was the earliest reaction from outside Rutherford's circle, where Bohr had spent some time as a "postdoc", and it revealed a vivid interest in the theory of the unknown author. "I thank you very much for sending me your highly interesting paper, which I had already read in the Phil. Mag.", Sommerfeld referred to the July-issue of this journal. "The problem of expressing the Rydberg-Ritz constant in terms of Planck's h has for a long time been on my mind. Some years ago I told Debye about it. Though for the present I am still rather sceptical about atomic models in general, calculating this constant is undoubtedly a great feat. [...] Will you also apply your atom model to the Zeeman effect?" (quoted in [Hoyer 1981, p. 123]).

The first part of this reaction refers to Bohr's derivation of a formula for the hydrogen spectrum

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

where ν is the frequency of a spectral line, N the constant that Sommerfeld called the Rydberg-Ritz constant, n and m integers ($n = 1, 2, 3 \ldots =$ the number that specifies a spectral series, $m = n+1, n+2, \ldots =$ the index within a series). $n = 2$ corresponds to the Balmer series with the spectral lines $H_\alpha (m = 3)$, $H_\beta (m = 4)$, etc. For the Rydberg-Ritz constant (which was previously known only as an empirical constant) Bohr's theory yielded

$$N = \frac{2\pi^2 me^4}{h^3},$$

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[1] "Meine Spektrallinien sind endlich in der Akademie in's Unreine gedruckt. In den Annalen werden sie in geläuterter Form erscheinen". Sommerfeld to W. Wien, 10 February 1916. DMA, NL 56, 010. Also in ASWB I. Wilhelm Wien and Max Planck served as editors of the *Annalen der Physik*.

[2] For the German reproduction of and commentary on these memoirs see [Eckert and Sommerfeld 2013].

with m = electron mass, e = elementary charge and h = Planck's constant. When Bohr had presented his model to Ernest Rutherford he had received a similar reaction. The ideas concerning the hydrogen spectrum are "very ingenious and seem to work well", Rutherford had praised this consequence of Bohr's model, but "the mixture of Planck's ideas with the old mechanics make it very difficult to form a physical idea of what is the basis of it" (quoted in [Hoyer 1981, p. 112]).

The latter part of Sommerfeld's reaction ("Will you also apply your atom model to the Zeeman effect?") hints at Sommerfeld's most recent research interest, the Paschen-Back effect. In 1912 Friedrich Paschen and Ernst Back had discovered that the splitting of spectral lines in a magnetic field changed at high field strengths in a characteristic way: the effect was described as a "magnetic transformation" such that Zeeman components, that were described as anomalous at weak field strength, merged into the normal Zeeman triplets at high field strength [Paschen and Back 1912]. Sommerfeld offered a simple explanation for this effect: if the quasi-elastic vibration of an electron around its mean position in an atom was no longer assumed as isotropic (as in Lorentz's classical theory for the normal Zeeman splitting) but as anisotropic with three slightly different frequencies along the axes of a cartesian coordinate system, then a magnetic transformation would occur when the field strength was so high that the differences of the oscillation frequencies were negligible [Sommerfeld 1913]. "These days I have conceived a work on the Zeeman phenomenon following Paschen-Back and I would like to know whether it is new", Sommerfeld asked Carl Runge, an expert on spectroscopy, in January 1913[3].

Others with whom he corresponded on these issues were Woldemar Voigt, an authority on magneto-optic theory, the astronomer Karl Schwarzschild and Paschen[4]. The quest for a theory of the Zeeman effect that was able to account for the discovery of Paschen and Back is also reflected in their publications [Schwarzschild 1914b; Sommerfeld 1914; Voigt 1913a,b,c]. Sommerfeld regarded Voigt's theory as an admirable effort to describe the facts, but he did not share Voigt's trust in the underlying physical model. "As long as we do not have a theory of spectral lines each theory of magneto-optics remains piecemeal."[5] In his own effort he just attempted to show "that Voigt's equations for the D-lines may be brought into a surprisingly simple form." [Sommerfeld 1914, p. 207].

Bohr's model must have appeared to Sommerfeld as a promising candidate for a theory of spectral lines, but with regard to the Zeeman effect it did not live up to his expectations. In a paper "On the Effect of Electric and Magnetic Fields on Spectral Lines", published in March 1914 in the *Philosophical Magazine*, Bohr expressed his belief that the Zeeman components could not be represented by a formula of the type of the hydrogen lines, i.e. as a difference of two terms [Bohr 1914, p. 519]. To make matters worse, the magnetic moment associated with the motion of an electron in the first Bohr orbit around a nucleus was one order of magnitude larger than the empirically determined "Weiss magneton". Bohr had no answer to the question how his model could be applied to magnetic phenomena – at least this was Sommerfeld's impression in June 1914. "Apparently there is much truth in Bohr's model", he wrote in a letter to Langevin, "and yet I believe that it has to be re-interpreted in a fundamental manner. At the moment I find it particularly disturbing that it yields a wrong value for the magneton."[6]

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[3] Sommerfeld to Runge, 17 January 1913. DMA, HS 1976-31. Also in ASWB I.

[4] This is evident from their correspondence in DMA, HS 1977-28/A,253, HS 1977-28/A,347, NL 89, 015 and SUB (Voigt and Schwarzschild).

[5] Sommerfeld to Voigt, 24 March 1913. DMA, NL 89, 015. Also in ASWB I.

[6] Sommerfeld to Langevin, 1 June 1914. ESPC, Langevin, L 76/53. Also in ASWB I.

Another phenomenon that became a challenge for Bohr's model was the Stark effect. By the end of 1913, Johannes Stark and Antonio Lo Surdo had independently discovered that the spectral lines of hydrogen are split in electric fields [Leone et al. 2004]. The first attempt to explain this splitting in terms of Bohr's model was made by Emil Warburg, the president of the Physikalisch-Technische Reichsanstalt (PTR) in Berlin. Warburg considered this effect as a phenomenon "which cannot be explained on the grounds of classical electrodynamics". But he also concluded that Bohr's model could not be applied to the Stark effect without some modifications [Warburg 1913, p. 1259 and 1266]. An attempt to explain the phenomenon in terms of classical electron theory was made by Schwarzschild who employed an analogy from celestial mechanics, the motion of a planet orbiting around two suns. If one sun is moved to infinity by simultaneously increasing its mass the planet moves in a gravitational field that corresponds to the motion of an electron around the hydrogen nucleus in the presence of a homogeneous electric field. However, neither the periods of the distorted electron orbits nor the number of split components agreed with the experimental observations [Schwarzschild 1914a]. Bohr corresponded with Warburg and Schwarzschild and dedicated a section to the Stark effect in his paper "On the Effect of Electric and Magnetic Fields on Spectral Lines" [Bohr 1914, pp. 512-518]. He assumed a deformation of the stationary circular orbits into ellipses that resulted in a splitting of singlets into doublets, with the frequency separation proportional to the electric field. In contrast to the Zeeman effect the splitting of spectral lines in electric fields appeared in agreement with the basic postulates of the Bohr atom, but there were not yet enough data for a detailed comparison between theory and experiment.

Sommerfeld closely observed these efforts. In summer 1914 Bohr was traveling through Germany. In Munich he used the opportunity for a presentation of his theory in Sommerfeld's colloquium. The entry in the colloquium book for 15 July 1914 reads "Bohr: On Bohr's model of the atom, in particular the spectra of helium and hydrogen"[7]. In this colloquium the question whether certain spectral lines belonged to hydrogen or helium must have been central. Prior to Bohr's model it was believed that hydrogen had two anomalous spectral series characterized by

$$\nu = N\left(\frac{1}{1.5^2} - \frac{1}{m^2}\right), m = 2, 3, 4\ldots$$

and

$$\nu = N\left(\frac{1}{2^2} - \frac{1}{(m+0.5)^2}\right), m = 2, 3, 4\ldots$$

The former was observed by Alfred Fowler in a tube that contained a mixture of hydrogen and helium, the latter by Edward Charles Pickering in the spectra of stellar nebulae. According to Bohr, however, these anomalous series for hydrogen could be regarded as normal series of ionized helium obeying formulae of the Balmer type. Multiplying numerator and denominator by 4 yields

$$\nu = 4N\left(\frac{1}{3^2} - \frac{1}{k^2}\right), k = 4, 5, \ldots$$

and

$$\nu = 4N\left(\frac{1}{4^2} - \frac{1}{k^2}\right), k = 5, 6, \ldots$$

In April 1914 Fowler agreed with Bohr that the spectral line

$$\nu = 4N\left(\frac{1}{3^2} - \frac{1}{4^2}\right)$$

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[7] Physikalisches Mittwoch-Colloquium. DMA, 1997-5115.

with the wavelength 4686 Å(=468.6 nm) belonged to ionized helium. It "must be concluded that the 4686 series is not due to hydrogen but to helium, as first suggested by Dr. Bohr from theoretical considerations", Fowler declared in the prestigious Bakerian lecture on 2 April 1914 [Fowler 1914, pp. 428-429].

Encouraged by this success, Bohr set out to extend his model. In order to account for minute corrections that appeared desirable for a better agreement with Fowler's experiments, he took into account elliptical electron orbits and a relativistic change of the electron mass – which resulted in a narrow doublet instead of a singlet. "Might not the disagreement", he asked Fowler, "in some way be connected with the doubling of the line?" (NBCW 2, p. 328). He published this extension of his model only in February 1915 in a paper "On the Series Spectrum of Hydrogen and the Structure of the Atom" [Bohr 1915b], but the fact that he mentioned it in his correspondence with Fowler already in April 1914 suggests that this was also a subject for discussion with Sommerfeld during his visit in Munich.

The Zeeman effect and spectral lines – a lecture in winter 1914/15

Sommerfeld was 45 years old when the First World War broke out. "Judging from what I have heard at the general headquarters, it seems that they are not very eager to make use of my services", he wrote to Schwarzschild in October 1914 with regard to the possibility that he would be drafted for military service. "If they leave me at home, it is just as well since I have never felt myself militarily strong." In this case he intended to lecture in the coming winter semester on "The Zeeman effect and spectral lines", as he announced to Schwarzschild with an attached page of shoptalk on the Zeeman effect[8]. He also corresponded with Paschen who communicated to him the most recent measurement on the anomalous Zeeman splitting[9]. Paschen also discussed with him the issue of the disputed 4686 Å line from the vantage point of experimental spectroscopy. "The question is still open and will be elaborated by one of my pupils who is now in the war. But I can tell you that Fowler's lines are also according to our experiments presumably helium lines."[10]

In the course of this winter semester Sommerfeld must have become convinced that the future of atomic theory belonged to Bohr's model – despite the Zeeman effect as a persistent bone of contention. What must have added to this conviction besides the issue of the "Pickering" and "Fowler" lines was another experimental investigation about the "fine decomposition" of Balmer lines in electric fields which Stark had published in October 1914. The number of components grew with the increasing index of the lines. Stark concluded that there must be several electrons in the hydrogen atom because he could not imagine that so many lines could be due to the oscillation of just one electron [Stark 1914, p. 444]. Sommerfeld had a different explanation. If the successive circular orbits in the Bohr atom are accompanied by a growing number of elliptic orbits of equal energy, then the transitions from a higher to lower energy coincide in a singlet; but this coincidence is removed when a disturbance such as an applied electric field deforms these orbits so that they have no longer equal energies. This was presumably the subject of a colloquium on 16 January 1915 when Sommerfeld talked "On the number of line decompositions in the Stark effect of hydrogen"[11].

Sommerfeld must also have communicated this idea to his assistant Wilhelm Lenz, then in the trenches at the western front, because Lenz congratulated him in April

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[8] Sommerfeld to Schwarzschild, 31 October 1914. SUB, Schwarzschild 743. Also in ASWB I.

[9] Paschen to Sommerfeld, 15 and 21 December 1914. DMA, HS 1977-28/A,253.

[10] Paschen to Sommerfeld, 7 February 1915. DMA, HS 1977-28/A,253.

[11] Physikalisches Mittwoch-Colloquium. DMA, 1997–5115.

1915: “I got excited about your discovery with regard to the Bohr model and the Stark effect, and I am very curious about the further progress.”[12] A month later Sommerfeld wrote in a letter to Wilhelm Wien: “During the past semester I obtained an interesting approach for the Stark effect from Bohr’s theory of the hydrogen lines.”[13] Immediately at the close of the winter semester he had written to Wien: “I have lectured on Bohr during this semester and am extremely interested in his theory as far as the war permits. Today’s 100 000 Russians, however, are even more beautiful than Bohr’s explanation of the Balmer series. I have marvelous new results in this regard.”[14]

Unfortunately these are the only contemporary utterances from winter 1914/15 and spring 1915 from which we may infer Sommerfeld’s route towards the extension of Bohr’s model. In summer 1915, he became committed to war research and to a Festschrift that was due by this time. As he wrote to Wilhelm Wien, “on the one hand problems of war physics and on the other a contribution to the Elster-Geitel-Festschrift have cropped up”[15]. The latter was titled “The general formula of dispersion according to Bohr’s model”, but it referred to Bohr’s model concerning the structure of molecules and not to Bohr’s model of the hydrogen atom [Sommerfeld 1915a]. Furthermore, Sommerfeld became excited by Einstein’s recent work on the general theory of relativity. At the end of the summer semester he wrote to Schwarzschild: “I have lectured this semester on relativity as presented by Einstein in his recent Berlin communication and am enthusiastic about it, almost as much as about Bohr in the preceding semester.”[16]

Two treatises for the Bavarian Academy of Science, 1915/16

By autumn 1915 several events prompted Sommerfeld finally to elaborate his extension of Bohr’s model. In August 1915 Bohr had submitted a paper “On the Quantum theory of radiation and the structure of the atom” which summarized the current achievements of Bohr’s model and indicated further applications [Bohr 1915a]. A paragraph on X-ray spectra (“high frequency spectra”), in particular, must have appeared to Sommerfeld as an intrusion in his own territory. X-ray spectroscopy was a pet research topic in Munich since the discovery of X-ray diffraction in 1912. Kossel had concluded in 1914 from an analysis of X-ray data that the electrons in atoms must be arranged in successive rings and that X-rays are emitted when an inner ring looses an electron. This suggested a close analogy between Bohr’s explanation of the spectral series in hydrogen and X-ray spectra [Heilbron 1967]. In November and December 1915 Sommerfeld and Kossel reported in the Munich colloquium on Bohr’s recent work and a recent doctoral dissertation on X-ray spectra, respectively[17]. On 24 November 1915 Paschen had written to Sommerfeld that he was now convinced “that Bohr’s theory is exactly correct except for the complicated structure of the lines 4686, etc”[18].

Sommerfeld’s extension of the Bohr model suggested an explanation for these lines as well as for the X-ray data. He must have elaborated it when he became aware of

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[12] Lenz to Sommerfeld, 10 April 1915. DMA, NL 89, 059.

[13] Sommerfeld to Wien, 3 May 1915. DMA, NL 56, 005. Also in ASWB I.

[14] Sommerfeld to Wien, 22 February 1915. DMA, NL 56, 005. Also in ASWB I. The remark about the 100,000 Russians refers to the defeat of the 10th Russian army in a battle in East Prussia when about 100,000 Russian soldiers became prisoners of war.

[15] Sommerfeld to Wien, 3 May 1915. DMA, NL 56, 005. Also in ASWB I. On Sommerfeld’s war research see [Eckert 2013a, chapter 7].

[16] Sommerfeld to Schwarzschild, 31 July 1915. SUB, Schwarzschild 743. Also in ASWB I.

[17] Physikalisches Mittwoch-Colloquium. DMA, 1997-5115.

[18] Paschen to Sommerfeld, 24 November 1915. DMA, HS 1977-28/A,253. Also in ASWB I.

Bohr's recent work. Perhaps he was afraid that Bohr would proceed along similar lines to those he had conceived in the preceding winter semester? Although there is no archival evidence for the precise timing, we may infer from a letter of Einstein that Sommerfeld elaborated his extension by November 1915. "You must not be angry with me that I respond to your friendly and interesting letter only today", Einstein wrote to Sommerfeld on 28 November 1915. He excused the delayed answer with his work on the general theory of relativity which had caused him "one of the most exciting, straining, but also most successful periods of my life". At the end of this letter he added: "I will now study your two treatises and send them back to you."[19]

A week later Sommerfeld presented the first of these treatises at a session of the mathematical-physical class of the Bavarian Academy of Science. "Yesterday I presented in the Academy a work on the Balmer series", he wrote to Wilhelm Wien on 5 December 1915, by chance his birthday. "I told you already some time ago in Würzburg about the quantized ellipses; in the meantime I have carried on this matter."[20] By the end of December he also informed Schwarzschild. "What I am doing? At the moment spectral lines full steam ahead and with fabulous results", he responded to Schwarzschild's request. "By quantizing the eccentricity of ellipses (in the same manner as the orbital motion) I show that to a series term $1/m^2$ belong m possible orbits; the associated frequencies coincide according to the usual mechanics, but differ somewhat according to the theory of relativity."[21]

The crucial step for this extension was not just to add ellipses to Bohr's circles and to make use of relativity theory – both had been considered already by Bohr – but to invoke an approach that allowed the quantization of several degrees of freedom. Sommerfeld resorted to a procedure that had been introduced by Planck at the Solvay Congress in 1911, when Planck had postulated $\int\int dq\,dp = h$ as the smallest phase space cell for the oscillators of his theory for black body radiation [Planck 1912, p. 99]. The q and p of Planck's theory were the coordinate and momentum of a one-dimensional harmonic oscillator. Sommerfeld's case concerned two-dimensional Keplerian motion, described in polar coordinates with an azimuthal (φ) and a radial (r) coordinate and the associated momenta p_φ and p_r, respectively. Sommerfeld's quantum condition amounted to integrals for each coordinate

$$\int p_\varphi d\varphi = nh$$

$$\int p_r dr = n'h$$

where the integration was taken over a complete orbit. If the radius was assumed as constant, the second integral vanished and the first reduced to the quantization of the angular momentum in circular motion as in Bohr's original model. If r was allowed to vary, the second integral described what Sommerfeld had called in his letter to Schwarzschild the "quantization of ellipses". He addressed this topic in the first treatise in a paragraph under the headline "quantum condition for the eccentricity" [Sommerfeld 1915b, p. 436]. In a preceding section he derived an expression for the energy of an electron in an elliptic orbit by quantizing only the angular momentum $p_n = \frac{nh}{2\pi}$. He obtained

$$W_n = -\frac{2\pi^2 me^4}{h^2n^2}\left(1-\epsilon_n^2\right) = -Nh\frac{1-\epsilon_n^2}{n^2}$$

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[19] Einstein to Sommerfeld, 28 November 1915. DMA, HS 1977-28/A,78. Also in ASWB I.

[20] Sommerfeld to Wien, 5 December 1915. DMA, NL 56, 010. Also in ASWB I.

[21] Sommerfeld to Schwarzschild, 28 December 1915. SUB (Schwarzschild 743). Also in ASWB I.

where N is the Rydberg constant and ϵ_n the eccentricity of the ellipse. Sommerfeld argued that ϵ_n varies continuously so that the difference of the energies in two Keplerian orbits cannot yield discrete spectral lines. In other words: allowing for elliptic motion with only one quantum condition did not work.

By adding $\int p_r dr = n'h$ as a separate quantum condition the total energy became discrete and dependent on two quantum numbers [Sommerfeld 1915b, p. 439]:

$$W_{n,n'} = -\frac{2\pi^2 me^4}{h^2}\frac{1}{(n+n')^2} = -Nh\frac{1}{(n+n')^2}.$$

Instead of Bohr's formula for the hydrogen spectrum

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

one obtained

$$\nu = N\left(\frac{1}{(n+n')^2} - \frac{1}{(m+m')^2}\right).$$

Thus the same spectral line could be caused by transitions between different circular and elliptic orbits with equal energies. The H_α-line from the Balmer series, for example, which originated in Bohr's model from a transition of the third to the second circular orbit, could now be generated by transitions from three orbits with the quantum sum $m+m' = 3$ to two orbits with the quantum sum $n+n' = 2$, that is $2\times 3 = 6$ transitions. Sommerfeld anticipated that not all of these transitions would be realized [Sommerfeld 1915b, p. 448]. Nevertheless this multiplicity was the virtue of his theory. It hinted at the line splitting in the Stark effect, because an applied electric field would remove the coincidence and thus yield a growing number of decompositions from H_α $(m+m' = 3)$ to H_β $(m+m' = 4)$, H_γ $(m+m' = 5)$, etc. Sommerfeld acknowledged that Bohr's explanation of the Stark effect yielded the correct order of magnitude for the shift of certain components. But Bohr's explanation only yielded doublets. It failed completely with respect to the feature which Sommerfeld's approach promised to explain: the growing number of decompositions. However, for the time being, Sommerfeld could not yet offer a quantitative theory of the Stark effect because he did not know how to apply the quantum condition for orbits which were distorted by the electric field [Sommerfeld 1915b, pp. 449-451].

It is perhaps needless to add that Sommerfeld's – like Bohr's – approach did not offer an explanation of the Zeeman effect. Another difficulty concerned the applicability to atoms with more than one electron. Sommerfeld anticipated the introduction of a third quantum number n'' for a third phase integral concerning the z coordinate which would amount to a spatial quantization [Sommerfeld 1915b, p. 453]. The final paragraph of this treatise addressed the problem of what coordinates had to be chosen for the phase integrals. For the treatment of Keplerian motion polar coordinates suggested themselves, but how to proceed in other cases [Sommerfeld 1915b, p. 455]?

Among these unsolved problems there was one for which Sommerfeld could offer a solution with far-reaching consequences. This was the subject of the second treatise. Sommerfeld presented it to the Academy immediately after the Christmas holidays on 8 January 1916. In this treatise he presented the relativistic theory of Keplerian motion. The orbit of an electron in this motion is no longer closed. Sommerfeld accounted for the deviation from the non-relativistic case with a factor $\gamma < 1$ (such that the precession of the perihelion during one orbit is $\frac{2\pi}{\gamma} - 2\pi$) and derived an expression for the energy of the relativistic Kepler ellipse. Here $n\gamma^2 + n'$ replaced the sum $n+n'$ from the non-relativistic case. The energy, which in the non-relativistic case depends only on the sum of two quantum numbers, now becomes different for each pair of different quantum numbers – with the result that previously coinciding transitions become decomposed and give rise to a fine-structure of spectral lines. Sommerfeld presented this result in the form of series expansions whose terms were proportional to powers of a dimensionless quantity $\alpha = (\frac{\pi e^2}{hc})^2 = 13.010^{-6}$ [Sommerfeld 1916a, pp. 469-470] (this was not yet the fine-structure constant; see below).

As a first application Sommerfeld elaborated the fine-structure splitting of the Balmer series (and corresponding series of hydrogen-like atoms). The non-relativistic series term with $n + n' = 2$ corresponds to the coinciding terms $n = 2, n' = 0$ and $n = 1, n' = 1$; in the relativistic case these terms no longer coincide so that all transitions from higher terms should be doublets corresponding to the term difference $W_{2,0} - W_{1,1}$. The associated frequency difference becomes in lowest order [Sommerfeld 1916a, p. 473]

$$\varDelta\nu = \frac{N\alpha B}{2^4}\left(\frac{E}{e}\right)^4 ,$$

where B is a constant [Sommerfeld 1916a, p. 463] and E is the nuclear charge (i.e. $E = e$ for hydrogen, $E = 2e$ for helium, etc.). The constant B accounted for an uncertainty about the limits of integration in the phase integral for the azimuthal motion in a precessing ellipse; Sommerfeld specified B only from hindsight in an appendix [Sommerfeld 1916a, p. 499]. He wished to show, however, that some of his conclusions were independent of this uncertainty, such as the ratios between different doublets [Sommerfeld 1916a, pp. 474-475]. The uncertainty was only resolved later by Schwarzschild. It no longer appears in Sommerfeld's refined version [Sommerfeld 1916b, p. 7].

For the experimental corroboration of these consequences Sommerfeld relied on Paschen's measurements. It was difficult to see the fine-structure splitting in the Balmer series because these lines appeared blurred even in high resolution spectrographs due to Doppler broadening. Nevertheless Paschen confirmed Sommerfeld's expectation. He had photographed "H_α und H_β as double lines" but regarded these as not satisfactory as long as it was not clear "whether the duplicity could not be due to some known or unknown effects (Stark effect, for example, as Bohr assumes it as possible)"[22]. While it was difficult to verify the doublet in the hydrogen lines, the factor $(\frac{E}{e})^4$ predicted a doublet sixteen times larger in the spectrum of the ionized helium. The disputed line $\lambda = 4686$ Å appeared as an ideal candidate for a test of Sommerfeld's fine-structure prediction. "I conclude that the complicated structure is due to the term $\frac{4N}{3^2}$", Paschen wrote to Sommerfeld in the same letter. But he still believed in Bohr's view that the orbit in the helium atom was distorted as a result of a Stark effect due to the complicated structure of the nucleus. Sommerfeld doubted this view and asked Paschen for a closer check[23]. Paschen immediately reacted and thanked Sommerfeld for "your highly interesting letter. So the discrepancy is theoretically required! There is nothing like a fine theory!"[24] Sommerfeld referred to this confirmation also in his treatise [Sommerfeld 1916a, p. 484].

The final part of this treatise is dedicated to consequences of Sommerfeld's fine-structure theory in the area of X-ray spectra. Following the discovery of X-ray diffraction by crystals in 1912 (see [Eckert 2012; Forman 1969; Jenkin 2001]) Henry Moseley had found in 1913 a formula for the emission of X-rays that resembled the Balmer formula and suggested an interpretation in terms of Bohr's model [Moseley 1913, 1914]. The source of X-rays is heavy atoms with many electrons that cannot be compared

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[22] Paschen to Sommerfeld, 12 December 1915. DMA, HS 1977-28/A,253. Also in ASWB I. For the problems with the hydrogen fine-structure see [Robotti 1986].

[23] Sommerfeld to Paschen, 29 December 1915. DMA, HS 1977-28/A,253. Also in ASWB I.

[24] Paschen to Sommerfeld, 30 December 1915. DMA, HS 1977-28/A,253. Also in ASWB I.

to the one-electron atom of Bohr's model. But in 1914 Walter Kossel inferred from absorption data of X-rays a ring structure of many-electron atoms which suggested a mechanism like that in Bohr's model [Heilbron 1967]. When an electron is lost from an inner electron ring, then filling the gap by an electron from an outer ring results in the emission of X-rays, just like the transition of an electron from an excited state in the hydrogen atom to a lower orbit causes the spectral lines of the Balmer series. Ivar Malmer, a doctoral student of the Swedish spectroscopist Manne Siegbahn, found that K_α, the strongest X-ray line, is accompanied by a weaker line; the frequency difference of these "K-doublets", as Sommerfeld called them, obeyed the same formula as the fine-structure doublets of hydrogen and ionized helium [Sommerfeld 1916a, pp. 493-494]. "The same settings as in hydrogen are met in the K and L series of X-rays", Sommerfeld reported to Schwarzschild. "I show that for all elements from $Z = 20$ bis $Z = 60$, where observational data are available, $\frac{\Delta\nu}{(Z-1)^4} = \Delta\nu_H$! $\Delta\nu$ = frequency difference in the X-ray doublets, $\Delta\nu_H$ = frequency difference in the hydrogen doublets."[25] Due to the "magnification factor" $(Z-1)^4$ the X-ray doublets of platinum or gold could be used for the determination of the barely measurable hydrogen doublet, Sommerfeld concluded at the end of this treatise [Sommerfeld 1916a, p. 498].

Towards the refined version, 1916

From the appendix to this treatise, dated 10 February 1916, it is apparent that Sommerfeld had good reasons to assert his priority for the extension of Bohr's model. In this appendix Sommerfeld addressed papers by Max Planck published in December 1915 on "The Quantum Hypothesis of Molecules with Several Degrees of Freedom" [Planck 1915a,b,c] which used the same quantization of phase integrals but fell short of Sommerfeld's results with regard to the detailed analysis of the spectra [Sommerfeld 1916a, pp. 498-500]. Einstein had informed Sommerfeld already in December 1915 that "Planck is also working on similar problems to you (quantization of the phase space of molecular systems). He is also working towards spectral issues."[26] Max Wien, a cousin of Wilhelm Wien, reported in the same vein about Planck ("competitor on spectral lines") from Berlin to Munich[27]. But when Sommerfeld sent his Academy treatises to Planck he received the reassurance that he should not be concerned about a rivalry. Planck decribed his recent effort as "only a little side-trip into a terrain that I had barely entered until now, by which I wished to direct the attention to the striking relations which one obtains between the structure of the phase space and Bohr's formulae... Now I see that this was unnecessary, for now the problem is with you in the best hands."[28] Planck was not primarily interested in Bohr's model or spectral lines. His main effort addressed a deficiency of his black-body theory which operated with one-dimensional oscillators as sources of radiation. Henri Poincaré had alluded to this deficiency when he asked Planck at the first Solvay Congress in 1911 how one had to quantize systems with several degrees of freedom. Planck's "side-trip" was an attempt to answer this question [Eckert 2010; Planck 1916].

"You will be interested to learn that Planck's quantization of the phase space agrees exactly with my approach", Sommerfeld wrote to Wilhelm Wien on the same day he added the appendix to his Academy treatise. "But Planck's explanation of the Balmer series is horrible and totally different from mine". Nevertheless Sommerfeld

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[25] Sommerfeld to Schwarzschild, 28 December 1915. SUB (Schwarzschild 743). Also in ASWB I.

[26] Einstein to Sommerfeld, 9 December 1915. DMA, HS 1977-28/A,78. Also in ASWB I.

[27] Max Wien to Sommerfeld, 4 January 1916. DMA, NL 89, 059.

[28] Planck to Sommerfeld, 30 January 1916. DMA, HS 1977-28/A,263.

regarded his work on "spectral lines" as not yet accomplished. "In the Annalen they will appear in refined form", he announced the further elaboration of his theory[29]. He also corresponded with Schwarzschild about Planck's approach: "I enjoyed very much the exact coincidence with Planck's structure theory of the phase space. Despite such different vantage points and so different modes of thinking (Planck careful and abstract, I somewhat ballsy and immediately aiming at what can actually be observed) exactly the same results!"[30]

The major issues that demanded to be addressed in the refined form was the Zeeman and Stark effects. The quest for a theory of these phenomena had originally prompted Sommerfeld's extension of Bohr's model – but was still unsolved. "This is now the hour for a true theory of the Zeeman effect, after the nature of the doublets has been recognized as due to different orbits", Sommerfeld wrote to Wilhelm Wien[31]. The main problem concerned the quantization of orbits which are deformed from the circular or elliptical shape. Sommerfeld received the decisive hint how to cope with this problem from Schwarzschild who suggested resorting to the Hamilton-Jacobi formalism and choosing action-angle variables for the quantization. "If one applies this procedure to the relativistic Kepler motion one obtains straightforwardly the results of your appendix which thereby becomes for me really compelling", Schwarzschild wrote to Sommerfeld on 1 March 1916 from a "business trip to Brussels" where he served as a scientific advisor in an artillery unit. "Furthermore this procedure provides a compelling approach for the Stark and Zeeman effects."[32] The quantization of phase integrals was thus transformed into a quantization of action variables. "On my return from Brussels I became convinced that my quantum approach is also in general agreement with that of Planck and that it is the true expression of what he actually means", Schwarzschild added a few days later. "Did you already assure yourself how it works with the Zeeman and Stark effects?"[33]

Sommerfeld was enthusiastic. "Although I am not familiar with your terms from general celestial mechanics (the unique angle variables w_k) I do believe that our views are not far apart from one another. What I have printed recently is of course no longer up-to-date." Thus he alluded to the appendix of his Academy treatise from February 10th[34]. Backed by Schwarzschild's confidence he entrusted the theory of the Stark effect to Paul Epstein as a subject for his habilitation. Since his arrival in Munich in 1910 Epstein had become an active member of Sommerfeld's circle. As a Russian citizen he was officially under arrest due to war-time regulations, but he was allowed to work in Sommerfeld's institute. Epstein had barely familiarized himself with the methods of celestial mechanics (in particular the problem of a planet moving in the field of two fixed centers) when Sommerfeld told him that Schwarzschild was also working on the theory of the Stark effect. "Now I was a little crestfallen, because I regarded this as a stab in the back", he recalled many years later. "You see, I knew already how the electron moves, and I knew how to do it. I got up at 5 o'clock the next morning and by 10 I had the formula. And then the same morning I brought it to Sommerfeld. And what do you know, the same afternoon he got a letter from

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[29] Sommerfeld to Wien, 10 February 1916. DMA, NL 56, 010. Also in ASWB I.

[30] Sommerfeld to Schwarzschild, 19 February 1916. SUB (Schwarzschild 743). Also in ASWB I.

[31] Sommerfeld to Wien, 31 December 1915. DMA, NL 56, 010.

[32] Schwarzschild to Sommerfeld, 1 March 1916. DMA, HS 1977-28/A,318. Also in ASWB I.

[33] Schwarzschild to Sommerfeld, 5 March 1916. DMA, HS 1977-28/A,318. Also in ASWB I.

[34] Sommerfeld to Schwarzschild, 9 March 1916. SUB (Schwarzschild 743). Also in ASWB I.

Schwarzschild, and Schwarzschild had the wrong formula. It was the same order of magnitude, but didn't agree on the positions of the lines"[35].

Schwarzschild and Epstein reached their goal almost simultaneously. Schwarzschild reported his success to Munich on 21 March 1916[36]. Sommerfeld responded three days later that Epstein had arrived at the same result, but in addition had calculated a line which was missing in Schwarzschild's result. "Epstein will publish a preliminary note in the Physikalische Zeitschrift. He will use this work later as a habilitation in Zurich. He should write to you himself. Of course, he has attended my lectures on spectral lines, etc.[37]. Epstein's paper arrived on 29 March 1916 at the *Physikalische Zeitschrift* [Epstein 1916]. Schwarzschild presented his theory on 30 March 1916 to the Prussian Academy of Science [Schwarzschild 1916]. But he could not enjoy it because he suffered from a rapidly worsening disease and died on 11 May 1916. "When I sent him this Spring my paper on the quantized ellipses his astronomical and physical interests were mightily excited", Sommerfeld wrote in an obituary. "In letters from the war that followed one another in short succession and from his sickbed at home he developed his views for me. [...] The unequaled ease of his perception and the depth of his view for analytical, physical and astronomical relationships rendered him a pathfinder in this still rather mysterious field as if he had been made for it" [Sommerfeld 1916c, pp. 945-946].

While Epstein and Schwarzschild elaborated the theory of the Stark effect, Sommerfeld received a letter of his assistent Wilhelm Lenz from the Western front in Northern France which added to the "refinement" of his theory in another respect. Lenz suspected that the final formula for the spectral lines of hydrogen in the relativistic case should amount to a law that represented the spectral series in a simpler way than Sommerfeld's complicated formulae. With "Because this law was not explicitly presented in your paper I have derived it myself", he introduced the result of his calculation[38]:

$$\nu = \frac{m_0 c^2}{h}\left\{\left[1+\frac{\alpha^2}{(n'+\sqrt{n^2-\alpha^2})^2}\right]^{-\frac{1}{2}} - \left[1+\frac{\alpha^2}{(m'+\sqrt{m^2-\alpha^2})^2}\right]^{-\frac{1}{2}}\right\}$$

with

$$\alpha = \frac{2\pi e^2}{hc}.$$

Sommerfeld duly acknowledged this contribution. In his treatise for the Academy "the clarity and closeness of the spectral formula was lost", he admitted in his refined paper in the *Annalen der Physik*, because he had resorted too early to series approximations [Sommerfeld 1916b, pp. 53-54].

Thus the fine-structure constant α entered and became apparent in its role in the relativistic splitting of spectral lines. With $\alpha \to 0$ the fine-structure formula became the simple formula of Bohr's model. In his Academy treatise Sommerfeld had chosen $\alpha = \frac{\pi^2 e^4}{h^2 c^2}$ for the series expansion. Lenz's $\alpha = \frac{2\pi e^2}{hc}$ not only restored the closed form of the "spectral law" but could be interpreted more physically as the ratio of an electron's velocity in the first Bohr orbit to the speed of light [Sommerfeld 1919, p. 244]. This constant had already occured in other contexts and sparked speculations. In Sommerfeld's fine-structure theory it made its appearance as a fundamental

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[35] Interview with Paul S. Epstein by John L. Heilbron, 25 May 1962. AHQP. Available online at http://www.aip.org/history/ohilist/4592_1.html.

[36] Schwarzschild to Sommerfeld, 21 March 1916. DMA, HS 1977-28/A,318. Also in ASWB I.

[37] Sommerfeld to Schwarzschild, 24 March 1916. SUB (Schwarzschild 743). Also in ASWB I.

[38] Lenz to Sommerfeld, 7 March 1916. DMA, NL 89, 059. Also in ASWB I.

spectroscopic constant. But it took some more years before α became a symbol for the mysteries of the quantum world. A "true understanding of the value of your constant", believed Heisenberg in 1935, "is still far in the future"[39]. More than fifty years later Richard Feynman considered it "one of the greatest damn mysteries of physics: a magic number that comes to us with no understanding by man" (quoted in [Kragh 2003, p. 395]).

In 1916 the fine-structure constant merely served to bring "clarity and closeness" to Sommerfeld's theory. Sommerfeld regarded the virtue of his theory first and foremost as being its capacity to explain spectroscopic measurements – and in this regard Paschen contributed most for the "refinement" of his theory. Paschen focused his work on precision measurements of "the helium line 4686"[40] and reported by the end of March 1916 "the solution of the picture puzzle of 4686"[41]. The theory put spectroscopy on a new basis, Paschen congratulated Sommerfeld, because it could be used now for the determination of fundamental constants of nature by spectroscopic means. "I do not know whether Planck's constant can otherwise be determined so precisely... Radiation measurements are certainly not precise enough. The agreement between H_α, the lines of lithium and now 4686 according to your theory is very fine indeed."[42] Paschen and Sommerfeld exchanged almost weekly long letters about the details of fine-structure measurements. "My measurements are now finished and are in wonderful agreement with your fine structures", Paschen wrote to Munich on 21 May 1916. "Without your theory these results would not have been found... If you publish your theory now in the Annalen I could refer to it"; he suggested a coordinated publication of their results.[43] He submitted his paper "On Bohr's helium lines" by the end of June 1916 [Paschen 1916]. Sommerfeld sent his paper "On the theory of spectral lines" one week later to the *Annalen der Physik*. He emphasized in particular the "exact corroboration of the fine structure at the helium lines of Paschen" and Paschen's suggestion to determine constants of nature by spectroscopic means, where "the characteristic constant of our fine structures $\alpha = \frac{2\pi e^2}{hc}$" would play an important role [Sommerfeld 1916b, pp. 80-94].

Outlook

Sommerfeld's colleagues reacted enthusiastically to his extension of Bohr's atomic model. "Your spectral analyses number among my finest experiences in physics", Einstein congratulated. "Only through them Bohr's idea becomes entirely convincing."[44] By and large, Sommerfeld's work was perceived as a corroboration of Bohr's model. Paul Ehrenfest, for example, added to his congratulation the regret that "this success helps to bring new triumphs to the Bohr model that for the time being is still so utterly cannibalistic."[45]

Bohr himself was most conscious what this extension meant for his model. "Sommerfeld's beautiful results fall exceedingly well in with my considerations", he confided to a close colleague and friend. He had just drafted a paper that aimed to put his theory on a more solid foundation. "But the form in which my paper was

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[39] Heisenberg to Sommerfeld, 14 June 1935. DMA, HS 1977-28/A,136. Also in ASWB II.

[40] Paschen to Sommerfeld, 10 March 1916. DMA, HS 1977-28/A,253. Also in ASWB I.

[41] Paschen to Sommerfeld, 28 March 1916. DMA, HS 1977-28/A,253.

[42] Paschen to Sommerfeld, 1 April 1916. DMA, HS 1977-28/A,253. Also in ASWB I.

[43] Paschen to Sommerfeld, 21 May 1916. DMA, HS 1977-28/A,253. Also in ASWB I.

[44] Einstein to Sommerfeld, 3 August 1916. DMA, HS 1977-28/A,78. Also in ASWB I.

[45] Ehrenfest to Sommerfeld, undated [April/May 1916]. DMA, HS 1977-28/A,76. Also in ASWB I.

written was much too narrow (or perhaps better too general) to allow simply to introduce Sommerfeld's results, and I am therefore contemplating to write an entirely new paper instead."[46] Bohr also thanked Sommerfeld most euphorically for sending him the two academy treatises which he immediately made known also to Rutherford and other colleagues in Manchester: "I do not think that I have ever enjoyed reading of anything more than I enjoyed the study of them, and I need not say that not only I but everybody here has taken the greatest interest in your important and beautiful results... The intention of writing all this is only to tell you how exceedingly glad I was to receive your papers before my own paper was published. I decided at once to postpone the publication and to consider it all again, in view of all for which your papers have opened my eyes."[47]

Bohr did not publish the paper mentioned in this letter. But the reference to this unpublished work hints at the role which Sommerfeld's articles played for Bohr's own extension of his theory. This became apparent only in 1918 with the first part of a comprehensive account "On the quantum theory of line spectra" where Bohr made the correspondence principle the uniform point of view for the further development of his ideas[48]. In the introduction, Bohr explicitly referred to Sommerfeld's papers and the ensuing work of Epstein and Schwarzschild as the starting point for this new stage in the quest for the atomic theory which ultimately paved the way for quantum mechanics.

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Abbreviations

ASGS	Arnold Sommerfeld. Gesammelte Schriften. 4 vols. Braunschweig: Vieweg, 1968.
ASWB	Arnold Sommerfeld. Wissenschaftlicher Briefwechsel. vol. I: 1892-1918; vol. II: 1919-1951. Edited by Michael Eckert and Karl Märker. München, Berlin, Diepholz: Deutsches Museum and GNT-Verlag, 2000 and 2004.
DMA	Deutsches Museum, Archiv. München.
ESPC	Ecole supérieure de physique et de chimie industrielles de la ville de Paris, Centre de ressources historiques, Paris.
NBCW	Niels Bohr Collected Works. 12 vols. North-Holland Publishing Company: Amsterdam, New York, Oxford, 1972–2006.
RANH	Rijksarchief in Noord-Holland, Haarlem.
SUB	Staats- und Universitäsbibliothek, Göttingen.
UAM	Universitätsarchiv, München.

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[46] Bohr to Oseen, 17 March 1916. Quoted in NBCW 2, p. 340.

[47] Bohr to Sommerfeld, 19 March 1916. Quoted in NBCW 2, p. 340. Bohr's letter was translated by his brother Harald into German and sent to Sommerfeld from Copenhagen. DMA, HS 1977-28/A,28. Also in ASWB I.

[48] See NBCW 3.

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