Suman Seth

Statement

and

Readings

"Memories and Matrices": Re-Thinking the "Crisis" of the Older Quantum Theory

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Abstract

"The history of science, to my knowledge," wrote Thomas Kuhn, describing the years just prior to the development of matrix and wave mechanics, "offers no equally clear, detailed, and cogent example of the creative functions of normal science and crisis." By 1924, most quantum theorists shared a sense that there was much wrong with all extant atomic models. Yet not all shared equally in the sense that the failure was either terribly surprising or particularly demoralizing. Not all agreed, that is, that a crisis for Bohr-like models was a crisis for quantum theory.

This paper attempts to answer four questions: two about history, two about memory. First, which sub-groups of the quantum theoretical community saw themselves and their field in a state of crisis in the early 1920s? Second, why did they do so, and how was a sense of crisis related to their theoretical practices in physics? Third, do we regard the years before 1925 as a crisis because they were followed by the quantum mechanical revolution? And fourth, to reverse the last question, were we to call into the question the existence of a crisis (for some at least) does that make a subsequent revolution less revolutionary?

Crafting the Quantum

Arnold Sommerfeld and the Practice of Theory, 1890–1926

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7 Crafting the Quantum: Sommerfeld, Bohr, and the Older Quantum Theory

Ich kann nur die Technik der Quanten fördern,
Sie müssen ihre Philosophie machen
—Sommerfeld to Einstein, 1922[1]

Kepler should have experienced today's quantum theory. He would have seen the boldest dreams of his youth realized, not, admittedly, in the macrocosm of the stars, but in the microcosm of the atom. The shell structure of the atom is even more wonderful than the cosmography longed for by Kepler. —Sommerfeld, 1925[2]

Technik and *Atom-Mystik*

A significant portion of chapter 6 sought to elucidate Niels Bohr's efforts in the early 1920s to "develop systematically the principles of quantum theory." This chapter is concerned with Sommerfeld's equivalent statement of purpose, offered, like Bohr's, in the first months of 1922. A letter to Einstein written in January reported the many successes of Sommerfeld's recent work and that of his students, including a young man in his third semester, Werner Heisenberg, who had just completed pioneering work in providing a model for the anomalous Zeeman effect. In spite of this, the situation was not ideal: "Everything works, but remains at the deepest level unclear." That, however, was not Sommerfeld's problem. Laying out the division of labor for the new physics, he wrote: "I can only advance the craft of the quantum, you have to make its philosophy." What it meant to craft the quantum, and more generally, what the physics of problems became in the Weimar period, is one of the questions considered below.

Before proceeding to an answer, however, a brief discussion of terminology is in order. In contemporary German, *Technik* is commonly accorded one of three different English equivalents: "technique," "technology," or "engineering." The phrase above has uniformly been translated as expressing Sommerfeld's preference for "the techniques of the quantum."[3] Yet "technique" in English has a connotation not necessarily intended in German, for it describes only "the mechanical or formal part of an art"; that part "distinct from general effect, expression, sentiment, etc."[4] A late-nineteenth-century text on music put it this way: "A player may be perfect in technique, and yet have neither soul nor intelligence."[5] Given Sommerfeld's defense of *Technik* against those who charged it with possessing "a smaller degree of scientific rigor" than their own disciplines and the importance of technical applications in his own work, one would hardly expect him to share this sentiment.[6] More generally, however, the formalistic implications of the word in English are less prevalent in the German. Grimm's nineteenth-century *Wörterbuch*, for example, offers the following definition: "the artistic or craft activity and the sum of experiences, rules, principles, and know-how according to which, through practice, an art or craft is pursued." Central to this understanding, as Norton Wise has argued in analyzing Helmholtz's use of the term, was a sense of the importance of an aesthetic sensibility for the *Techniker*.

Aesthetics was essential for Sommerfeld's work on the quantum theory of spectral lines. The same man who would speak of an anti-philosophical, "nuts and bolts" approach to the quantum would also, in the same period, wax lyrical about the harmonious "number mysteries" that a study of spectral lines allowed one to glimpse.[7] The preface to the first edition of *Atombau* would, one suspects, make any hard-headed technician blush:

> What we are nowadays hearing of the language of spectra is a true "music of the spheres" within the atom, chords of integral relationships, an order and harmony that becomes ever more perfect in spite of the manifold variety. The theory of spectral lines will bear the name of Bohr for all time. But yet another name will be permanently associated with it, that of Planck. All integral laws of spectral lines and of atomic theory spring originally from the quantum theory. It is the mysterious organon on which nature plays her music of the spectra, and according to the rhythm of which she regulates the structure of the atoms and nuclei.[8]

On the other hand, Sommerfeld reacted with palpable fury when the *Süddeutsche Monatshefte* contacted him—one suspects after reading utterances like the one above—to write an article on astrology. "Doesn't it strike one as a monstrous anachronism," he raged, "that in the twentieth century a respected periodical sees itself compelled to solicit a discussion about astrology? That wide circles of the educated or half-educated public are attracted more by astrology than by astronomy? That in Munich probably more people get their living from astrology than are active in astronomy?" In spite of having "no illusions" about his ability to hold back the growing tide of irrationalism that threatened to wash away the remnants of a reasoning European culture, Sommerfeld pledged to "throw myself decisively against it."[9]

Yet it was not only the editors of newspapers and the "half-educated public" that perceived Sommerfeld as espousing an irrational or at least arational approach to the physical world. His colleague Wilhelm Wien, a professor of experimental physics at Munich, snidely referred to Sommerfeld's work not as *Atomistik*, but *Atom-Mystik*, a phraseology that Wien's students apparently adopted.[10] This private (or at least intra-faculty) jibe became public when Wien delivered a rectoral address, at Munich in 1926, on the "Past, Present and Future of Physics." Among the lecture's main topics was the modern atomic theory, and the developments that followed the introduction of the Bohr model. It did not mention Sommerfeld—almost certainly in the audience at the time—by name, a reproach (even an insult) in itself.[11] Even more telling, Wien closed with a discussion of the hope offered by Schrödinger's new wave theory of removing talk of mysticism from quantum-theoretical research:

> Now Schrödinger is trying to ascribe the whole numbers of the quantum theory to similar characteristic vibrations [*Eigenschwingungen*], the actual physical meaning of which admittedly still remains dark. If that were really to succeed, then the special role which whole numbers play in the quantum theory would also here be eliminated, also here number mysticism would be supplanted by the cool logic of physical thought; probably not to the joy of everyone. Because mysticism exercises a greater attraction on many minds than the cold and clinical mode of thought of physical contemplation. I am far from wanting to attack mysticism as such. There are many areas of spiritual life from which mysticism cannot be shut out, but it does not belong in physics. A physics in which mysticism rules or only participates leaves the ground from which it draws its strength and ceases to deserve the name.[12]

If Wien took the talk of mysticism in Sommerfeld's work at face value, and perceived in it a disturbing and widespread tendency toward the denial of the "cool logic of physical thought," Max Born took a more cynical (if thereby more supportive) position. On the occasion of Sommerfeld's sixtieth birthday, Born remarked:

> He occasionally speaks with gentle coquetry of number mysticism in spectral laws; but he means by that nothing philosophically dark, but only the statement that so far one has still not come directly behind these laws. The word should be once again a lure for spurring on young brains to restless research; because he who is in Sommerfeld's school, for him is mysticism only there to be vanquished.[13]

How are we to judge the meaning of Sommerfeld's talk of *Zahlenmystik*: as a fine aesthetic sense of harmony in physics, as mere pandering to forces of irrationalism, or as a wily way to win students to one's school? The answer, I suggest here, is by understanding it as a constitutive element of the *Technik* of the quantum. To see this requires a close examination of the practices and methodologies of Sommerfeld's work in the 1920s. It was on these practices and methodologies that Pauli, a former member of the Sommerfeld School, commented in 1945 on the occasion of receiving a Nobel Prize for the discovery of the exclusion principle:

> At that time there were two approaches to the difficult problems connected with the quantum of action. One was an effort to bring abstract order to the new ideas by looking for a key to translate classical mechanics and electrodynamics into quantum language which would form a logical generalization of these. This was the direction which was taken by Bohr's Correspondence

> Principle. Sommerfeld, however, preferred, in view of the difficulties which blocked the use of the concepts of kinematical models, a direct interpretation, as independent of models as possible, of the laws of spectra in terms of integral numbers, following, as Kepler once did in his investigation of the planetary system, an inner feeling for harmony. Both methods, which did not appear to me irreconcilable, influenced me.[14]

In this account, Sommerfeld's emphasis on Keplerian harmony is neither window dressing nor a flight from science and reason. It is, rather, a direct response to the problems of the quantum theory. Bohr's use of the correspondence principle, in contrast, since it relied on the translation of ideas between the classical and quantum realms, becomes an indirect method of dealing with similar difficulties.

Pauli's words, of course were written two decades after the events he was describing, but there are good reasons for seeing in them a clue to Sommerfeld's own understandings of the methods he would employ. Consider, for example, the only mention of number mysteries in the text of the first article in which he would use that term.[15] There the turn to a study of numerical regularities is portrayed as precisely a result of the failure of model-based analysis;

> The musical beauty of our number table is thereby not derogated at all by the fact that it for the time being represents a number mystery. In fact, I see at the moment no way toward a model-based [*modellmässig*] explanation, neither of the doublet-triplet phenomena, nor of their magnetic interaction. In the same sense all spectroscopic laws were, until a few years ago a number mystery.[16]

Why Sommerfeld should have felt, around 1919, inspired to abandon a *modellmässig* approach, and how his contemporaries reacted to such a move, are the subjects of this chapter's second section. The third section explores and seeks to explicate his reaction to Bohr's use of the correspondence principle, while the final section examines the variegated problems taken up by members of the Munich school from the end of the war to the mid 1920s. There, as we shall see, *Technik* would take on a double meaning, as students aided Sommerfeld in his quantum craftsmanship and continued to explore the technological problems that had been so central to the school before 1918.[17]

Unsettled Questions of Atomic Physics

In the early weeks of 1920, Sommerfeld began receiving letters congratulating him on the publication of the first edition of *Atombau.* Theoreticians and experimentalists alike lauded the achievements of the text. David Hilbert spoke of reading the "masterly" volume "with daily increasing joy." Hans Beggerow cited the book's "clear and simple" language, which proved its character as a "true classic." Pieter Zeeman claimed that it read like a "thrilling novel."[18] Yet not all of Sommerfeld's correspondents were entirely positive. Although Max Born insisted that little should be changed, and that the book was "marvelous as it is," he also offered some rather pointed criticisms. Sommerfeld, he suggested, had indulged in an excess of "local patriotism," overemphasizing the achievements of those connected to his own school at the expense of those—including Bohr—whose methods differed from those regularly deployed in Munich. In addition, Born criticized the representation of the state of the field that the book appeared to put forward: "You represent some matters in such a way that the lay reader must believe that everything is in order; but that is certainly often not the case. E.g. the molecular model of H_2, etc., as well as the whole theory of Röntgen-spectra." Alfred Landé, Born reported, had recently informed him that the precise opposite was the case: that the theory of x-ray spectra was in disarray. "Would it not be good to emphasize the doubts a little more?"[19]

Sommerfeld took the criticisms to heart. Later editions contained much more detailed and sympathetic portrayals of Bohr's successful utilization of his "analogy principle." The second edition, completed in September 1920, also made more of an effort to bring to light areas of the theory that remained either incomplete or positively confusing. In advance of the publication of the text, Sommerfeld penned a two-page essay for the *Physikalische Zeitschrift* on "Unsettled Questions of Atomic Physics," noting that such questions outnumbered those that had, thus far, been fully and satisfactorily answered.[20] The two areas that Sommerfeld emphasized were both ones in which he had toiled since his first papers on the Bohr-Sommerfeld quantization conditions: the relationship between hydrogenic and non-hydrogenic spectra, on the one hand, and the question of the "topology of the atomic core"—explored through data on Röntgen spectra—on the other.[21] His failure, at least in his eyes, to produce a model-based understanding of these two subjects, one that could provide a dynamical foundation for the empirically based regularities that Sommerfeld *could* derive, would lead by 1922 to his abandonment of the *modellmässig* approach for all aspects of the atomic theory, excepting only, perhaps, the model of the hydrogen atom with which he had begun.

Fine Structure, the Zeeman Effect, and the Birth of a Number Mystery

Sommerfeld began his discussion by laying out the basic theory used to understand atomic spectra. Referring the reader to the diagram reproduced here as figure 7.1, he reminded them of the fact that emission series of spectral lines were produced when an electron moved from a higher to a lower energy level, giving off electromagnetic radiation of a frequency determined by the expression $\Delta E = h\nu$. Each line was thus, according to the "principle of combination," made up of two terms, corresponding to the energy of the initial and final states. The differences between energy levels may be organized into various series, denoted by the letters *s, p, d, b* (sharp, principal, diffuse, Bergmann). Each energy level was described by a quantum number, *m*, made up of the sum of the fixed "azimuthal" quantum number *n* and the variable "radial"

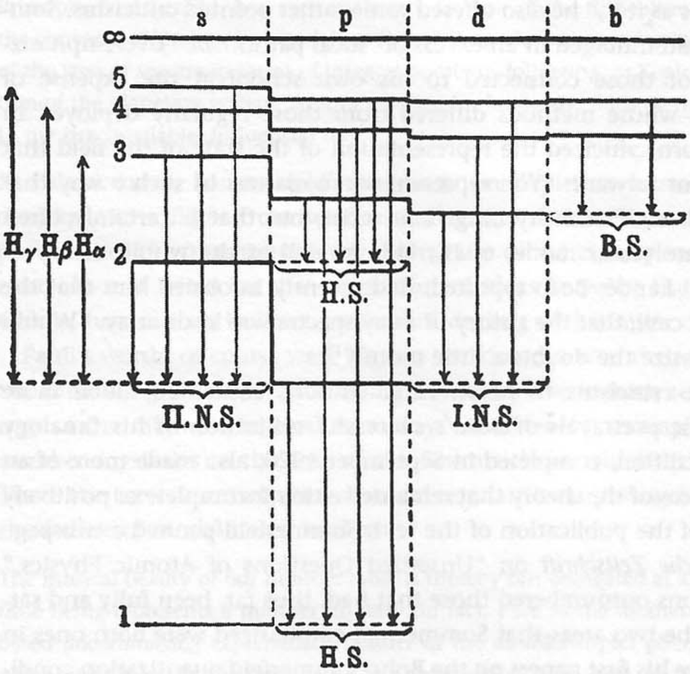


Figure 7.1

Energy-level diagram for sodium. Source: Sommerfeld, "Schwebende Fragen der Atomphysik." *Physikalische Zeitschrift* 21 (1920): 619–20.

quantum number *n*' (i.e., *m* = *n* + *n*'). In Sommerfeld's formulation, *n* = 1, 2, 3, 4 for the *s, p, d, b* series, respectively.[22]

Not all transitions from a higher to a lower energy level are allowed. A "selection principle" offered, in Sommerfeld's words, "an essential supplement to the principle of combination, through which its boundlessness is contained and its practical value raised."[23] The only jumps possible were those for which $\Delta n = \pm 1$ *or* 0. In other words, an electron could move from its current level to a lower, neighboring level (or a level beneath it in the same series), but to no others. The origin of the differing heights of energy levels with the same value of *m* was explained by the action of electrons closer to the nucleus than the transitioning electron. Their negative charge "shielded" part of the nucleus's positive charge, resulting in a diminution in the attraction experienced by the outer electron from the normal Coulombic force; a diminution that depended for its exact value on the spatial organization and motions of the inner electrons. Since a hydrogen atom only possesses a single electron, one would assume that no such alteration to the Coulomb force could occur, and, in fact, corresponding energy levels for all four series were the same, i.e., *ms* = *mp* = *md* = *mb*. Only when one took relativistic effects into account did a step-like structure for hydrogen's energy levels emerge, and with it came the element's characteristic spectroscopic fine structure. Where, in the absence of a relativistic mass correction, all transitions from the third energy level to the second overlapped, now three distinct transitions were possible, producing a triplet: $3d \rightarrow 2p$, $3s \rightarrow 2p$, $3p \rightarrow 2s$. As Sommerfeld phrased it, hydrogen's fine structure corresponded to "non-hydrogenic gross-structure."[24] The link was a neat one, but it left an obvious question unanswered, for no analogue in the hydrogen spectrum existed that corresponded with the observed fine structure of non-hydrogenic elements. The *p* and *d* levels in the diagram had to be imagined as yet further divided, and "for the model-based meaning of these subordinate levels no satisfactory explanation has yet been given."[25] Sommerfeld held out hope that some of Bohr's recent work might aid the situation, but his closing remarks on the subject served merely to indicate the field's deep lack of certain knowledge. "That we have here to do with completely new matters," he wrote, "is shown, in particular, by the anomalous Zeeman effect, which is bound up with the existence of such more subtle divisions of energy levels."[26]

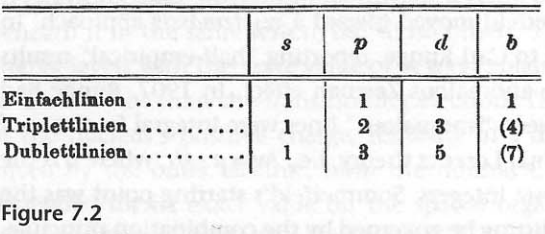
If model-based understanding of non-hydrogenic fine structure was, indeed, inextricably tied to a concomitant understanding of the splitting of lines in a magnetic field, then Sommerfeld was well aware of the problems ahead. In 1916, flushed with the success of his extensions of Bohr's model, he had turned his hand to the question that had first occupied his mind after reading of Bohr's results in 1913: the Zeeman effect. The result was strikingly disappointing. In common with Debye, who had taken up the problem independently, Sommerfeld showed that a quantum calculation of the size of line splitting led to a result that "does not coincide with the result of the classical theory, but is very close." The splitting induced by the magnetic field in Sommerfeld's treatment was equal to a whole number times the classical value obtained through Lorentz's electron theory.[27] The relativistic Zeeman Effect, to Sommerfeld's considerable surprise, was no different from the non-relativistic, meaning that the existence of a relativistic fine structure seemed to have no effect on the results.[28] The calculation could say nothing about the line multiplicities of the anomalous Zeeman Effect.

To deal with that problem, Sommerfeld moved toward a *gesetzmässig* approach. In the middle of August 1919, he wrote to Carl Runge, reporting "half-empirical" results that relied on "Runge's rule" for the anomalous Zeeman effect. In 1907, Runge had determined that the separations between "anomalous" lines were integral fractions of the separations predicted by the original Lorentz theory, i.e., $\Delta\nu = a \cdot s/r$, where a is the Lorentz separation and both s and r are integers. Sommerfeld's starting point was the suggestion that the size of the line splitting be governed by the combination principle. Then $\Delta\nu = \Delta\nu_1 - \Delta\nu_2$, where the terms on the right-hand side correspond to the splittings of the first and second terms respectively. If $\Delta\nu_1/a = s_1/r_1$ and $\Delta\nu_2/a = s_2/r_2$, then

$$\frac{\Delta\nu}{a} = \frac{s_1 r_2 - s_2 r_1}{r_1 r_2} = \frac{s}{r}.$$

Sommerfeld termed the result his "magneto-optic splitting rule," arguing that it demonstrated that the "Runge number" (*r*) of each term combination was made up of two components: the Runge numbers of the first and second terms.[29]

The first public discussion of this new spectroscopic rule came the following month, when Sommerfeld lectured in the southern Swedish town of Lund.[30] A version of that paper was published early the next year in *Die Naturwissenschaften* under the title "A Number Mystery in the Theory of the Zeeman Effect."[31] The "mystery" was less the rule itself than the implications Sommerfeld drew from it. The article reproduced a table that Sommerfeld had included in his letter to Runge, laying out the empirically determined Runge components. (See figure 7.2.) All single lines displayed values corresponding to the normal Zeeman effect ($r_1 = 1$) and all *s* terms in doublets and triplets were, Sommerfeld claimed, "single without exception, according to general spectroscopic experience."[32] These observations provided the data for the first row and column of the table. Runge numbers for lines corresponding to a combination of an *s* term and a *p* term, he noted next, were 2 = 2 × 1 for triplets, and 3 = 3 × 1 for doublets, numbers that accordingly filled out the *p* column of the table. According to data supplied recently by Paschen, it was further reported, Runge numbers for lines related to the combination of a *p* and a *d* term were 6 = 2 × 3 for a doublet, and 15 = 3 × 5 for a triplet. "With these numbers," he wrote, "we fill in the third column of our table and see a wonderful number harmony complete itself thereby." This number harmony could then, itself, provide the basis for predictions of future, experimentally determined, Runge numbers. "No one will doubt," Sommerfeld claimed, with perhaps excessive optimism, "that we must complete the fourth column with the numbers 4 and 7," corresponding to a pattern of increasing ordinal numbers in the second row and increasing odd numbers in the third.[33] The measurable Runge number for doublets made up from *b* and *d* terms should then be 12, for triplets, 35. Of the reason for these numbers, and the origin of the doublets and triplets, Sommerfeld could say nothing.



	s	*p*	*d*	*b*
Einfachlinien	**1**	**1**	**1**	**1**
Triplettlinien	**1**	**2**	**3**	**(4)**
Dublettlinien	**1**	**3**	**5**	**(7)**

Figure 7.2

Sommerfeld's number table for Runge components. Source: Sommerfeld, "Ein Zahlenmysterium in der Theorie des Zeeman-Effektes," *Die Naturwissenschaften* 8 (1920): 61–4.

"The actual cause for the doublets and triplets," he confessed to Runge, "and therefore also the cause of the anomalous Zeeman effect is still unclear to me. Only this much is certain, that in all whole-numbered relationships, quanta are involved [*stecken*]."[34] The paper on number mysteries promised that a "more fundamental" discussion of his results would follow in the *Annalen*, yet that article also eschewed an extensive model-based analysis. "General Spectroscopic Laws, in Particular a Magneto-optic Splitting Rule," published in 1920, began with a description of the hopes of the teens—all too soon to be dashed—that the hydrogen spectra would provide the key to lines in the spectra of all elements. After hydrogenic spectra had been explained, Sommerfeld noted somewhat wistfully, it had seemed only a short step until one could treat non-hydrogenic spectra along the same lines, "for example, tracing the doublet of the *D* lines to path differences in the atomic model." But nature had not proved so accommodating, and for the explanation of the line structure of series other than the Balmer series hydrogen, Sommerfeld wrote, "provides no clue."[35] He continued:

> Thus it is, that at the moment we are at a loss with the *modellmässigen* meaning of the line multiplicities of the non-hydrogenic elements, in spite of repeated efforts from various sides. All the more valuable are all the lawful regularities [*Gesetzmässigkeiten*] that present themselves empirically for the line multiplicities, above all when they are of such a radical and simple kind as those here at hand.[36]

The intention of the article in general was to further explicate several such known laws, and to introduce several new ones. In particular, the magneto-optic splitting rule "unveils a harmony of whole-numbered relationships of a purity that will even surprise those accustomed to the modern quantum theory."[37] There was more than harmony at stake here, however, for the new empirical laws were of both a theoretical and a practical importance as well, corresponding, Sommerfeld seemed to suggest, to the needs both of experimental and theoretical physicists. "The practical significance of multiple lines for the classification of spectroscopic series is well known," he wrote. "The theoretical significance of the line structures for the model-based investigation of the atom will doubtless be no less. We may promise for our magneto-optic splitting rule, apart from a theoretical also a practical importance for the meaning and ordering of the complex Zeeman effect."[38] It could serve, he opined later in the paper, as a "pointer [*Fingerzeig*] toward the correct interpretation of the observations."[39]

Sommerfeld's discussion served to locate the search for model-based explanations—as opposed to those based on empirical regularities—at some point in the future. It was not that models were to be removed from physics altogether, but that, since they had proved less useful than the direct search for regularities in empirical data, their use should be postponed. Spectral laws were concrete, atomic models conjectural. The five sections of the paper then laid out five distinct rules, none of which relied on the Bohr model. The first, Sommerfeld designated as "the law of permanence of multiplicities." It had long been known that elements in the same column of the periodic table displayed similar patterns of line splitting. Sommerfeld wanted to add to this rule the "until now little noticed fact" that the patterns of *p*-term and *d*-term splitting were identical for any given element: If the *p* term was a doublet, for example, then so, too, was the *d* term. The second rule, an extension of the already-enunciated "selection principle," sought to provide a rationale to explain why not all transitions between *d* lines and *p* lines were observed. Transitions denoted by broken lines in figure 7.3 were allowed by the selection principle (since here $\Delta n = 1$), but did not occur in reality. Sommerfeld's suggestion was that another quantum number was involved, one that obeyed its own selection rule. If the azimuthal quantum number was assigned to the angular momentum of the entire atom—its "external rotation"—then "the distinguishing characteristic of the various *d* and *p* terms must be, rather, an inner quantum number, perhaps corresponding to a hidden rotation. Of its geometric significance we are quite as ignorant as we are of those differences in the orbits which underlie the multiplicity of the series terms."[40] Assigning, for the inner quantum number, the values written to the left of each line—beginning with the highest values of *n* for that line—the selection principle for the outer quantum number holds here, too. The number can change by ± 1 or 0, but by no more. Re-emphasizing the fact that no geometrical or model-based representation of the inner quantum number was being offered with this rule, Sommerfeld emphasized again its "rather formal"

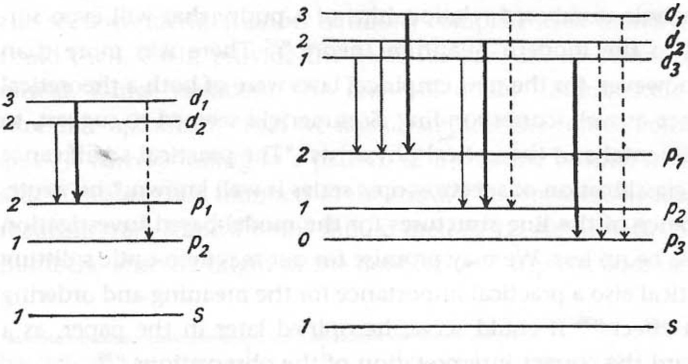


Figure 7.3

Transition diagrams for doublets (left) and triplets (right). Broken lines represent transitions possible in terms of the selection rule for *n*, since here $\Delta n = 1$. Such transitions, however, are not observed; hence Sommerfeld's suggestions that an additional selection rule, corresponding to an "inner quantum number," was in effect. Source: Sommerfeld, "Allgemeine spektroskopische Gesetze, insbesondere ein magnetooptischer Zerlegungssatz," *Annalen der Physik* 63 (1920): 221–63 character:

> I would not like to refrain from pointing out that, in transferring our selection principle to the "inner" quantum number and by the choice of the latter, we have proceeded rather formally. The physical fact is the exclusion of certain term combinations; that the cause of this is to be sought in quantum conditions appears certain to me. But the assumption that these quantum conditions have the same form as with the external quantum number is somewhat arbitrary.[41]

The basic form of rule three had been put forward by Sommerfeld and Walter Kossel in 1919, and was termed by them the "spectroscopic displacement law."[42] It held, in essence, that the spectrum for an element that had been ionized (i.e., had lost an electron) displayed the same splitting pattern as the un-ionized elements in the column preceding it in the periodic table; further, in numerical terms, it was best compared with the element immediately preceding it in the table. As Sommerfeld noted, the rule had a simple model-based explanation. Since one could take it as "empirically guaranteed" that the line character of an element depended solely on the number of its external (valence) electrons, then the removal of an electron should clearly produce line patterns like those of elements with one less electron in the outermost ring. Yet, as Sommerfeld continued, the "theoretical origin" of this rule "touches only on the most general lineaments of the model of the atom, on the incrementally increasing number of external electrons. Of the specific interpretation of the series terms…and of their allocation to the quantum numbers 1, 2, 3, 4 it is completely independent."[43] If *modellmässig,* that is, the rule drew barely, if at all, on the dynamical specificities of the Bohr model. So, too, with the fourth spectroscopic law, which extended a rule first put forward by Johannes Rydberg. The Swedish physicist had noticed that elements with an odd number of valence electrons characteristically produced doublet systems, those with even valence, triplets. Suggesting that the same logic should apply to ionized atoms, Sommerfeld outlined his "exchange law," which held that if an un-ionized element displayed a doublet in its arc spectrum, then its singly ionized form would display a spark-spectrum triplet, and vice versa.[44]

The fifth and final rule was the magneto-optic splitting law, which Sommerfeld introduced in terms similar to those used in his paper in *Die Naturwissenschaften.* Two new columns had been added to the number table: four further bracketed terms "developed only through analogy, not by observation." The table, he wrote, "is perhaps the most perfect example of those number harmonies which the new theory of spectra has bestowed upon us. It represents, for the time being, as I have noted elsewhere, a "number mystery." In fact, our table is of an essentially empirical origin and theoretically just as little understood as the origin of the line multiplicities more generally. Only so much appears to be certain: that the integral harmony of our Runge numbers has its final cause in the action [*Walt*] of hidden quantum numbers and quantum relations."[45]

In noting the similar language used to describe the lack of understanding of the geometrical significance of the inner quantum number and of the theoretical origin of Sommerfeld's number table, Forman has suggested that what ties the paper on "General Spectroscopic Laws" together is "a state of ignorance, conceived as a transitive relation connecting the complex structure with the anomalous Zeeman effect." "We are as ignorant," he argues, "of the significance of the inner quantum number as we are of the cause of the complexity of the spectral terms, and that is precisely how little we understand the cause of the Runge denominators of the terms."[46] Certainly, Sommerfeld made no bones about the extent of his ignorance, but a more charitable (and also more accurate) reading might note that there are not two but five parts to the paper, and all five hold in common their avoidance of dynamical, model-based explanations in favor of empirically based rules. In other words, ignorance about causes was traded for a functionalist understanding of regularities within phenomena. Finding no way to proceed using the theoretical tools he had been so instrumental in developing, Sommerfeld gave up the search for *modellmässig* foundations in order to develop a praxis—or craft—involving "half-empirical" *Gesetzmässigkeiten*.

The shift away from his earlier approach to the quantum theory of spectral lines was a dramatic one. Gone was the realist emphasis on dynamical model building. However, in its place was not, as one might expect, a Planckian emphasis on trans-historical, transcendental, purely theoretical principles. Indeed, in many ways the opposite was the case, since experimental data was not the end but the starting point of Sommerfeld's analysis. Yet an important resource for the formulation of what might be termed his aesthetic phenomenology is not hard to find. In 1913, while reworking Voigt's coupling theory of the Zeeman effect, Sommerfeld laid particular emphasis—as, indeed, did Voigt himself—on the phenomenological character of the theory. The particular values of the coupling coefficients of the mutually bound electrons were all drawn from empirical data, and no attempt to explain the cause of the coupling on electromagnetic grounds was offered. (See figure 7.4.) As Voigt put it, his investigation "restricts itself to the phenomenological level and is therefore satisfied with offering the necessary *preparatory work* for the later formulation of a model for the extremely complicated processes via an explanation of the quantitative relations which underlie the properties of the different degrees of freedom. In any case, the proof of the fundamental significance of the *cyclic coupling of the degrees of freedom* may be regarded as the *beginning* of the construction of a model for the explanation of recent observations."[47] For Sommerfeld, this conclusion was far too weak. The numerical relations between the coupling coefficients—brought to light in a particularly clear manner by his simplification of Voigt's equations—seemed to point to a more concrete result[48]:

> The simplicity and symmetry of these equations is highly suggestive with regard to the problem of the construction of an atomic model. Herr Voigt has remarked this already in the context of his general hypothesis of cyclic coupling; it applies to a greater extent to the simplified representation of the specific case of D-line coupling given here. The appearance of three roots of unity as weighting factors seems to point to a ring in which three electrons follow one another

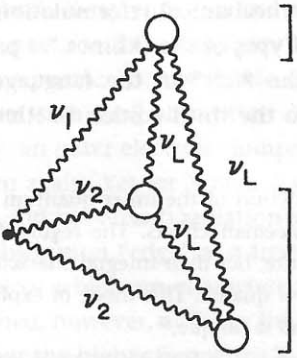


Figure 3. The Voigt-Sommerfeld Model for the Sodium D-Lines.

In a magnetic field the three electrons (circles) are coupled harmonically to a fixed center with frequencies ν_1 and ν_2 and to each other with frequencies ν_L, the Larmor frequency. In zero external field $\nu_L = 0$, the internal coupling disappears, and the electron generates an internal field $\mathbf{H}_i$ oriented along $\mathbf{k}^*$. The core is oriented along the resultant of H and $\mathbf{H}_i$.

Figure 7.4

Voigt's coupling model for the anomalous Zeeman effect. Source: David C. Cassidy, "Heisenberg's First Core Model of the Atom: The Formation of a Professional Style," *Historical Studies in the Physical Sciences* 10 (1979): 187–224.

equidistantly.…The number 3, corresponding to Runge's rule, plays the determining role in these equations; it is the only parameter of our equations. One may well suspect that with other atomic constructions and correspondingly altered types of Zeeman phenomena, other whole numbers will enter in some fashion that is also designated by Runge's rule. Perhaps the phenomenological study of the Zeeman effect after the fashion of Herr Voigt offers the most secure means for the building up of the structure of the atom; in this respect, the example of the D line's remarkably simple, number-theoretical *Gesetzmässigkeiten* gives us hope.[49]

Where Voigt, in other words, postponed model building, for the most part, to some future date, Sommerfeld saw phenomenology-based equations as the starting point for an immediate discussion of the nature of atomic structure. The more such equations were simplified, he concluded, "the closer we can expect to come to a real understanding of them and therewith to a certain insight into the atomic processes to which they correspond."[50]

Five years later, as the anomalous Zeeman effect seemed to provide many more questions than answers, Voigt's more cautious approach clearly seemed much more appealing. Writing to Zeeman at the beginning of 1920, Sommerfeld lamented Voigt's recent death, noting that the reference to the "musical beauty" of the number table in his *Zahlenmysterium* paper had been directed toward his former colleague. It is surely no coincidence that Sommerfeld's first paper after his complete conversion to a *gesetzmässig* method was his "Quantum mechanical reformulation of Voigt's Theory of the Anomalous Zeeman effect of the Types of the D Lines," a paper that sought to provide "the adequate expression of the facts" in the language of the quantum theory.[51] The first page of the preface to the third edition of *Atombau*, completed a month later, made his position clear:

> I attach particular importance to the introduction of the inner quantum numbers and to the systematic arrangement of the anomalous Zeeman effects. The regularities that here obtain throughout are primarily of an empirical nature, but their integral character demands from the outset that they be clothed in the language of quanta. This mode of explanation, just like the regularities themselves, is fully established and is unique.[52]

The only doubts that can arise, he concluded, are those "with respect to the interpretation in terms of the models."[53]

Rings, Cubes, and the *Ellipsenverein:* X-Ray Spectra and Atomic Structure[54]

In 1924, the year in which the fourth edition of *Atombau* appeared, Sommerfeld published an article in the *Annalen* on "The Theory of Multiplets and Their Zeeman Effect." As had become common by then, his introductory remarks included a methodological discussion, outlining his reasons for deferring model-based analysis for some point in the future. This element of his work is now familiar to us, but Sommerfeld's identification of the exemplar of his new approach was more novel:

> In the present state of theory, it seems to me to be most secure to put the question of model-based meaning in the background and to first bring the empirical relations to their simplest arithmetical and geometrical form. This rejection [*Verwahren*] has proven itself, e.g. in the theory of Röntgen spectra. While the specific models (circular rings, *Ellipsenverein*, cubes) have proven themselves to be unfruitful, the half-empirical systematics of Röntgen spectra, based on the principle of combination and selection rules, has led to valuable and secure results. We will proceed here, in the question of term structure, in a similar manner.[55]

The idea that the understanding of X-ray data might provide a model for the visible spectrum was one that had been unthinkable only five years previously. Early in 1919, Sommerfeld had written to Bohr of his exasperation with the problem. "I find it genuinely difficult to advance with the Röntgen spectra. There is much too much that is hypothetical in the assumptions about the position and occupation of the rings." Instead, he reported, "I have turned again more toward the visible spectra, about which I have received new material from Paschen."[56] In July he told the experimentalist Manne Siegbahn of recent lectures he had given on the problems of Röntgen radiation, "where certainly so much still lies in darkness."[57]

No doubt part of the vehemence of Sommerfeld's reaction stemmed from the frustration of hopes raised when he had first taken up the question of X-ray spectra in relation to Bohr's model in 1915.[58] A year before, Kossel had put forward a model that seemed to explain both X-ray emission and absorption data simultaneously. The feat was an impressive one, for the asymmetry between the two processes for Röntgen radiation had been a puzzle. For the visible spectrum, Bohr's model provided an easy explanation for emission and absorption as inverse phenomena: in absorbing a quantum of energy, an outer electron "jumped" to a virtual orbit; in emitting energy, it leaped back down again. Yet for X-rays, a given metal, which emitted its K_α line at a frequency $\nu = \nu_{K_\alpha}$, did not absorb radiation at the same frequency. There was, rather, a lower limit (an absorption "edge" at a frequency higher than any observed K lines for that metal), below which no characteristic K-ray absorption was possible. Once that limit was reached, however, all K-ray lines seemed to appear simultaneously (that is, not merely K_α, but the higher frequency K_β and even the newly observed K_γ). Kossel interpreted this result as implying that the frequency of the absorption edge, ν_K, was a measure of the ionization energy of the K shell. A metal, struck by high-energy cathode rays, according to this model, ejected an electron from the K shell. An electron from the L shell then dropped down to give the K_α line. Röntgen emission spectra, in other words, were only produced in the aftermath of ionization. This explanation implies, of course, that (since $E = h\nu$) $\nu_{K_\alpha} = \nu_K - \nu_L$ ($h\nu_L$ being the ionization energy of the L shell), a result that experiments appeared to verify. The identification of two L absorption edges then implied the existence of two L shells.[59]

Sommerfeld combined these ideas with his own relativistic extension of Bohr's model. Assuming the presence of a single electron in an L orbital (orbits designated, beginning with that closest to the nucleus, K, L, M, N,...), he envisioned it revolving about both the nucleus and any electrons in lower orbits. This resulted in an effective reduction of the nuclear charge, Ze—and hence the Coulomb force—which Sommerfeld represented by the term $(Z - l)e$. Since he had already explained the relativistic origin of a fine-structure doublet for hydrogen (of width $\Delta\nu_H$), he now had a near-equivalent explanation for the existence of the observed L doublet and could apply his previous results to determine a value for its size, $\Delta\nu$. To first approximation,

$$\Delta\nu = (Z - l)^4 \cdot \Delta\nu_H.$$

Including higher-order terms and comparing the more precise expression with experimental data for $\Delta\nu$ for elements ranging from lead ($Z = 46$) to uranium ($Z = 92$),[60] Sommerfeld calculated the value of the screening constant, $l = 3.5$. The result was both remarkable and perplexing. On the one hand, since l appeared to be the same for all elements across a significant part of the periodic table, this would suggest that they shared the same electron structure for their innermost regions—a gratifying result for anyone interested in *Atombau*. On the other hand, Sommerfeld's reasoning would suggest, as he himself admitted, that the value of l should be integral: regardless of their arrangement, n electrons inside the relevant orbit should reduce the effective nuclear charge by *ne*, not by a fractional amount. "How to explain this in terms of the model," Sommerfeld wrote, "remains open."[61]

That was not the only problem to face this first attempt at tackling X-ray spectra. If the problem of the "nuclear charge defect," as Sommerfeld would term it, seemed to depend for its answer on a reconsideration of the dynamical specificities of Bohr's model, a difficulty with the "combination principle" appeared to strike at the most fundamental assumption of Bohr's analysis. Since the frequency of any spectral line was to be obtained from the "combination" of two orbits, of energy E_1 and E_2 ($\nu = (E_2 - E_1)/h$), this could also be understood as a transitive property. Consider a transition from the *N* to the *L* orbital (the line $L_{\alpha'}$ in Sommerfeld's notation) and another from *M* to *L*. Since $(L - N) - (L - M) = M - N$, one should be able to calculate the frequency of the line corresponding to a transition from an *N* to an *M* orbital solely on the basis of data on the other two lines.[62] Empirically, however, the difference on the left-hand side was calculated to be 133.6 for uranium, while the lowest experimentally determined value for a transition from any *N* to any *M* orbital was measured to be 233.5. Similarly, since $(L - O) - (L - M) = M - O$, the two terms on the left-hand side should provide a measure for the frequency corresponding to a transition from an *O* to an *M* orbital. Instead, the data from the *L* series gave a difference equal to 350.7 for uranium, while the highest experimental value was 274.2. Sommerfeld wrote: "We must, therefore, declare that the combination principle for Röntgen radiation fails at precisely the place where it could be most precisely verified."[63]

A paper read to the Bavarian Academy in early November supplied, as its title suggested, a number of extensions to the original quantum theory of spectral lines, but had little concrete to offer concerning the two defects discussed above.[64] Completing a detailed calculation of the energy levels of quantized elliptical orbits near the nucleus, Sommerfeld nonetheless had to conclude that his original suggestion for the reason behind the non-integral value of the screening constant—the effect of "external" electrons—didn't enter into the picture. "The external electron ring," he wrote, "therefore produces no trace" of such a value.[65] Without actually performing the calculation, Sommerfeld suggested that the problem may have lain in the assumption of co-planar rings. Tilting the orbits in relation to one another—"stepping from the planimetry to the stereometry of the atomic core"—held out a hope of explaining the screening values: "important natural constants that are characteristic for the constitution of all elements of the natural system."[66] Sommerfeld's calculation offered no insight into the cause of deviations from the combination principle either. Again, all that could be supplied was a suggestion for future work. Attempting to determine the effect of orbits aligned so that they intersected those of external electrons might serve the purpose, but Sommerfeld was more than a little vague on details. "One can say perhaps," he wrote with more optimism than certainty, "that at least in a qualitative respect, the way has been pointed toward the explanation of the apparent deviations from the combination principle."[67]

There the matter rested until the final months of the war, when Sommerfeld once again took up the question of "Atomic Structure and Röntgen Spectra." The paper opened with a description of the continuing effort to explain the origin of the nonintegral value of l. Accepting that it was apparently impossible to derive the right value while assuming that a single electron orbited around a bunch of its fellows who screened it from the full nuclear charge, Sommerfeld noted attempts by both Bohr and Moseley to incorporate the possibility of multiply occupied rings, evenly spaced in a circular orbit. Of course, such an explanation could not work for Sommerfeld's elliptical orbits: rotating electrons equally spaced around an ellipse under a Coulomb force will not be stable. If, however, one imagined n electrons on n identical ellipses, with each ellipse spaced at an angle of $360/n$, then—assuming that each particle begins its motion at the same position—the electrons will trace out paths such that, at any moment, each stands at the corner of a regular n-sided polygon. This was the famous *Ellipsenverein*. Since a circle may always be drawn that touches all the corners of a regular polygon, the electronic motion may be envisioned in terms of a single circular orbit, expanding and contracting—indeed, pulsing—around the nucleus. A footnote to the description of this rather elaborate structure sought to deflect the obvious criticisms. "For my feeling," wrote Sommerfeld, "the artful interlocking of the n electronic paths in our 'Ellipsenverein' is nothing unnatural; I see much more a sign therein for the high harmony of motion that must rule within the atom."[68] (See figure 7.5.)

The question of the spatial orientation of electrons within orbits having been solved, Sommerfeld could turn toward what had become the central questions that many looked to X-ray spectra to answer. How was an atom structured? How many electrons were to be found in how many rings around the nucleus, and how was this structure related to the organization of the periodic table of elements? One might suspect, for example, that each ring corresponded to a row of the table and thus that the lowest, the K ring, could hold two electrons, the L and M rings eight each, the N ring 18, and so forth. While Sommerfeld had pursued other problems for the years between 1916 and 1918, several researchers had sought to determine the occupancy number of each ring by calculating its dynamical stability within the overall planetary model of the atom. None had been entirely successful.[69] Debye, undertaking one of the first analyses, arrived at the unconvincing result that, in a transition from the L to the K ring, the latter went from containing two to containing three electrons, while the former dropped from one to zero. Sommerfeld offered his own calculations as "essentially a theoretical basis" for results obtained by Jan Kroo, who had come up with the decidedly more appealing result: $K = 3$, $L = 9$. Kroo had taken the simple tack of writing down an expression for the energy difference between an atom in which the K ring contains $p - 1$ electrons and the L ring q electrons, and an atom where a transition has occurred, and the K ring has p electrons, the L ring $q - 1$. Determining the frequency corresponding to this energy (which, of course, must be the frequency of the

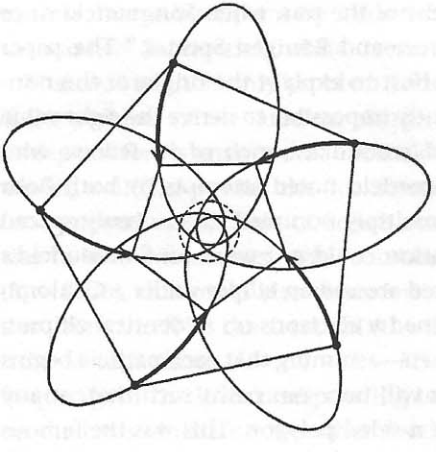


Figure 7.5

Sommerfeld's *Ellipsenverein*. "These ellipses are traversed by the q electrons in such a way, the same for each, that all the q electrons pass through the corresponding aphelia and perihelia at the same moment, respectively. If the electrons are joined up by a sequence of straight lines, then the latter will at every moment constitute a regular polygon (of q sides) which alternately contracts and expands. It is clear that in this pulsating polygon the repulsions exerted on one electron by all the remaining electrons must by symmetry give a resultant which passes through the nucleus...." Source: Sommerfeld, *Atomic Structure and Spectral Lines* (1923).

K_α line), Kroo fitted the data to his theoretical expression to obtain the numbers above. Sommerfeld claimed that he would "found mathematically the theory of the multiply occupied electron rings" but his actual achievement was rather more modest. What he could demonstrate was that one could essentially ignore the contribution of external rings when calculating the value of K_α, an assumption implicit in Kroo's analysis.[70] However, he ruefully acknowledged, "in further pursuit of the problem a series of difficulties emerge, which will possibly compel the foundation of the theory to be reformulated."[71] Of leading importance among those difficulties were, once again, the nuclear charge and combination defects, for which the *Ellipsenverein* could offer little cure.

Sommerfeld's report on the paper to Bohr was less than enthusiastic. "I find many difficulties here, particularly with the combination principle. The aim of determining the number of electrons in each ring appears to me still to lie in the far distance."[72] The sentiment stayed with him, as we have seen, into the new year. Although a diagram of the *Ellipsenverein* would be included in the first three editions of *Atombau*, so too would challenges of it, the elaborations of critiques gaining in length with the years.[73] Thus it was that atomic structure and X-ray data should be at the heart of the second of Sommerfeld's "unsettled questions of atomic physics." By 1920, when the paper was published, a series of results had appeared challenging the stability of "pancake" models with electrons arranged in co-planar rings.[74] It seemed necessary to consider atomic structure as a three-dimensional problem. Although he had, at first, appeared more resigned to than convinced by the arrangement proposed by Alfred Landé, with electrons in the second shell at each of the eight corners of a cube, by early September 1919 Sommerfeld had come to regard the die-shaped shell as the "salvation" of the theory of Röntgen spectra.[75] The religious fervor did not last long. The open question that he took up the next year was whether spectral data confirmed the details of the model. The simple answer was no, but an explanation was at hand. One need not conclude that the cubical picture was false, only that "the cube did not remain a regular cube."[76] If the *L* shell had the form of a die, then a single electron orbiting in the *M* shell would deform its shape, causing the Coulomb force acting upon it to change. There was room to hope that calculations (difficult though they might be) that dealt with orbits around this shifting three-dimensional structure might better accord with the results of experiment.

Sommerfeld was not the one to undertake such calculations. His own approach to Röntgen spectra began to take on the shape of his work on the anomalous Zeeman effect, being completed at the same time. Just as 1920 marked the point at which he began to elaborate a series of "half-empirical" laws for understanding the visible spectrum, the same year saw his turn toward an increasing use of selection principles in his analysis of X-ray data. Bohr's response to Sommerfeld's results, soon to be published as "Remarks on the Fine-Structure of Röntgen Spectra" was enthusiastic and captures Bohr's clear realization of the methodological distinction Sommerfeld was making between empirical regularities and model-based accounts:

> I was extremely interested in what you reported in your letter. The *Gesetzmässigkeiten* in the Röntgen spectrum that you mention are wonderful, and one cannot doubt that you have grasped the kernel of the problem. How one can represent it all in terms of a model [*modellmässig*] in its details and how one can overcome the difficulties associated with the limited space in the core of the atom is another story, about which I also feel—the more I try to think about it—that one still comprehends so little that scarcely any ground for skepticism may be found therein.[77]

The most important parts of the paper dealt with the application of the selection principle to the fine structure of the various series within X-ray spectra. Recent dissertation work by one of Siegbahn's students, W. Stenström, had revealed the existence of 1, 2, and 3 absorption edges in the *K*, *L*, and *M* series respectively, a fact that Sommerfeld immediately took as evidence that the splitting of the orbitals was governed by the same rules as in the hydrogen spectrum. If the quantum sum for the *M* level, for example, was accorded the value $n + n' = 3$ (in a manner analogous to the hydrogen triplet), then three energetically distinct orbits are possible: a circle and two ellipses. Similarly, the *N* level would be, in fact, a quartet, as depicted in figure 7.6.[78] Applying

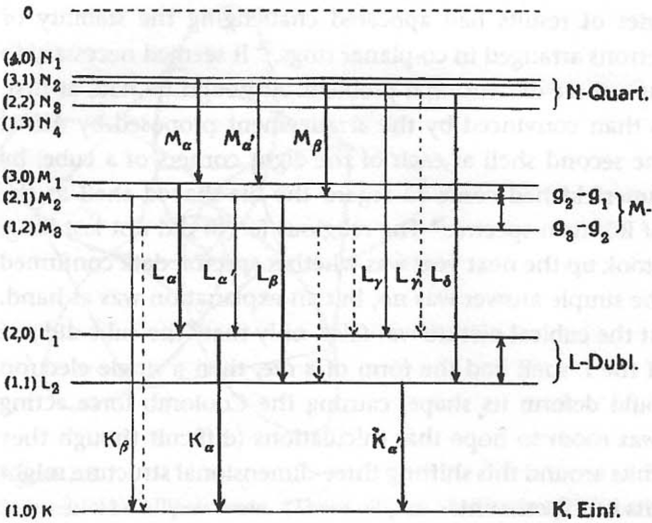


Figure 7.6

Splitting levels, based on absorption-edge and emission data. Source: Sommerfeld, "Bemerkungen zur Feinstruktur der Röntgenspektren I," *Zeitschrift für Physik* 1 (1920): 135–46.

the same selection principle deployed in his paper on spectroscopic laws, certain orbits—those for which the rule $n = \pm 1{,}0$ was not obeyed—could now be disallowed, *a priori*. Coupling this principle with an "intensity rule," derived by Bohr's assistant H. A. Kramers, which held that more intense lines were to be found in transitions where $\Delta n = +1$ than when $\Delta n = -1$ or 0, Sommerfeld could immediately explain a result which he had been emphasizing for some time. From his earliest papers on the topic, he had argued that the size of the *L* doublet was not given by the difference between the lines L_α and L_β—the two strongest lines in the *L* series—but by the difference between L_β and the weaker line $L_{\alpha'}$. One could now see why: pairs of strongest lines held neither their starting nor their end state in common.[79] Applying the same logic to the *M* series, it is clear that the difference between measured values for the second-strongest line M_β and the weaker $M_{\alpha'}$ should give the size of the gap between two of the lines of the *M* triplet ($M_1 - M_2$). Stenström's work offered an independent measure of this quantity, as the difference between two of the *absorption* edges of the series, which he labeled $g_2 - g_1$. The empirical match between the two quantities was remarkably close. For both uranium and thorium, the difference was less than 1 percent.[80]

Sommerfeld was now using a similar methodology for his work on both the Zeeman effect and X-ray spectra, but modeling had not yet been abandoned entirely for the latter problem. In 1918, he had predicted, on *modellmässig* grounds, the existence of a not-yet-observed partner to the known K_β line. In 1921, precision measurements carried out by another student of Siegbahn's, E. Hjalmar, appeared to confirm the fine structure of the line and Sommerfeld returned to his earlier analysis. The argument was a simple one. The energy of a transition was calculated as the difference between the energy of the atom before and after an electron moves from a higher to a lower orbit (or the reverse, in the case of absorption). For a transition from the *M* to the *K* orbital, this should have two components. One will simply be the energy difference between the two levels. The other component will come from the effect of the transition on the two orbitals associated with the *L* doublet. An extra electron in the K shell adds to the negative charge shielding the intermediary *L* orbitals from the nucleus and each will thus expand, changing the net energy of the atom. For Sommerfeld, however—and this point would prove crucial—the elliptical and circular orbits of the *L* doublet were not to be found within the same atom. The point was essential when considering the *Ellipsenverein,* otherwise the elliptical orbits corresponding to $n + n' = 1 + 1$ would cut into the circular orbit, with its evenly spaced electrons. By 1921, Sommerfeld had little faith in his "elliptical complex," but the notion that different kinds of orbits corresponded to different "species" of atoms remained: "One kind of atom, in which the more common L_1-level rules, gives the main line, β; the other kind of atom with the more rare L_2 level gives a neighboring line, β'." The point was reiterated in the article's final line: "One must always keep in view the fact that the processes, which we relate to the emission of β' and β", in either case, even if they occur in the very same element, must take place in different atoms (atoms of the L_1 or L_2 states)."[81]

The removal of this single plank from the overall structure of Sommerfeld's model-based argument caused the entire edifice to fall. An addition at the proof stage of the article read: "The last remark stands in contradiction to the latest results that Mr. Bohr has indicated in his letter to *Nature* of February 17 of this year. How the rest of the preceding remarks agree with Bohr's new viewpoint cannot, at present, be gauged."[82] Bohr's four-page letter, outlining how the correspondence principle could be used to determine the details of atomic structure, had shaken the work of the Sommerfeld school to its foundation.[83] "Your comment that Bohr has battered in like a bomb," he wrote to Landé in March, "is true for Munich as well. I received a copy of his letter to Nature from Bohr. We must thoroughly relearn [*umlernen*]."[84] To Bohr himself he raved that the letter "clearly signifies the greatest advance in atomic structure since 1913."[85] In fact, Bohr's letter was light on details, serving more as a promissory note for a paper to follow, but Sommerfeld took from it one essential claim: all orbitals, of whatever shape, that corresponded to a given element, had to be found within a single atom of that element. How profound was the effect of this realization may be easily discerned within the pages of the third edition of *Atombau.* Although the first and second editions had already sounded a skeptical note about the *Ellipsenverein,* the discussion in the third served to bury not only it, but the very project of atomic model building altogether. After describing the functioning of the interlocking ellipses, Sommerfeld noted that "a number of weighty objections speak against the truth of this picture." A few lines below he would list these objections:[86] first, as J. M. Burgers had noted, the ellipses meant to model the *L* shell actually intersected the path marking out orbits in the smaller K shell (the broken circle in the diagram)[87]; second, the coplanar arrangement was problematic, since it was unclear how the electrons were to be made to confer distinction on one plane over another; third, Landé's solution—a cubical arrangement—will not work either, since the question of the shape of the atom once one of its electrons is removed in the excited state is unclear. "But the most serious objection to polygonal as well as to polyhedral symmetry," Sommerfeld wrote, was the fourth:

> ...in order not to destroy the symmetry we should have to assume that the elliptical and circular modes of motion occur in *different* atoms, and that, accordingly, *one* part of the atom exemplifies the L_1 level, *another* part the L_2 level. Now in addition to the L_1 and L_2 level there is also an L_3 level. Moreover...there are 5 *M* levels and not less than 7 *N* levels.... But if we distribute L_1 and L_2 among different atoms we must also do the same with L_3, and with the *M* and *N* levels. Hence, we should have to postulate not two, but at least 1.3.5.7 = 105 different species of one and the same atom, corresponding to the possible combinations of the various levels with one another. That is already absurd in itself.[88]

The "intermediary doublet" explanation of the fine structure of the line had depended entirely upon this "absurdity." Now, as Sommerfeld phrased it, the theory "falls to the ground" with the conclusion "that the orbits that give rise to the different levels must actually all occur in the same atom." The credit for his realization of the necessity of this about-face was granted entirely to Bohr. "This conclusion," he acknowledged in a footnote, "is entirely contradictory to the view that the author held formerly, and was maintained in earlier German editions of this book. But it coincides with the views of Bohr expressed in his letter to *Nature*.... According to Bohr, it is an indispensable condition for the stability of the atom that the orbits of the various shells be interlocked, in a manner similar to that depicted for the *K* and *L* orbitals in [the figure of the *Ellipsenverein*]."[89] Along with the now-defunct intermediary doublet theory went any hope of explaining either atomic structure or the specificities of hard-won quasi-empirical expressions in a *modellmässig* fashion, yet Sommerfeld refused to regard this loss pessimistically:

> ...there can be no such pronounced symmetry as we assumed in the grouped ellipses or in the cubic arrangement. The problem of the arrangement of the electrons within the atom, regarded from an elementary point of view, becomes hopeless. It seems equally hopeless to explain the defect in the nuclear charge namely $s = 3.50$ in an elementary and pictorial manner.... [Yet] our formula for the *L* doublet does not hereby lose any of its practical value. It cannot, indeed, be regarded as an equation that has been derived from theory, like the formula for the hydrogen doublet, but it stands as an empirical equation that has been brilliantly confirmed.[90]

A sense of optimism, in fact, characterized the 1922 edition of *Atombau*. Sommerfeld declared in his preface that he let the text out of his hands with a "somewhat easier conscience" than he had for previous editions. Much had seemed "unripe and uncertain" in 1919 and, of course, the fields of theoretical and experimental spectroscopy were still in a state of "violent ferment" three years later. Yet the focus on *Gesetzmässigkeiten* allowed much greater hope that the claims of the present would be upheld in the future. For the case of Röntgen spectra, Sommerfeld noted, *modellmässig* interpretation "has been left out almost entirely. Whatever the further researches of Bohr may reveal to us concerning the shell structure of the atom, I feel certain that nothing will be changed in the laws...here described."[91] The point was true, moreover, for almost all of the subject matter of the book: "[T]he way in which the facts of Röntgen spectra, of term multiplicities, of Zeeman effects, have been put together, half-empirically and half by means of the quantum theory, will presumably remain unaffected by later developments. Bohr's recent far-reaching ideas will, indeed, add much that is new, but will not throw doubts on what appears to be established."[92]

In Praise (and Defense) of *Gesetzmässigkeiten*

Given his outspokenness with regard to the "unique" nature of his mode of explanation, it is perhaps unsurprising that Sommerfeld's method met with mixed responses. Max Born, in early 1923, professed to be both supportive and admiring, even if he felt himself unable to emulate his colleague's achievements. "Unfortunately," he wrote, "I do not have your ability to read such connections out of empirical spectral data, but must feel my way forward slowly on the path toward the gradual cleaning up and clarification of principles."[93] After the publication of the fourth edition of *Atombau* in 1924, both Wolfgang Pauli and Erwin Schrödinger wrote letters of effusive praise, each emphasizing in particular the avoidance of model-based explanations. By that time Pauli had become convinced that modeling was entirely inappropriate for the needs of the quantum theory, and clearly saw in Sommerfeld a solution to contemporary problems:

> I found it particularly beautiful in the presentation of the complex structure that you have left all *modellmässig* considerations to one side. The model idea now finds itself in a difficult, fundamental [*prinzipiellen*] crisis, which I believe will end with a further radical sharpening of the opposition between classical and quantum theory....One now has the impression with all models, that we speak there a language that is not sufficiently adequate for the simplicity and beauty of the quantum world. For that reason I found it so beautiful that your presentation of the complex structure is completely free of all model prejudices.[94]

Schrödinger was less critical of other approaches than the characteristically blunt Pauli, but no less admiring, admitting that it "remained incomprehensible to him" that Sommerfeld should have been able to draw such fundamental laws from "not at all so very rich factual materials" without a "proper [*eigentliches*] model." "I have trouble," wrote Schrödinger, "slowly clarifying to myself the admittedly really complicated building up of these whole-number formulas, and you've incorporated them into the observational material so that they now sit as tightly as a guard's uniform!"[95]

If some found the avoidance of models worthy of high praise, others found Sommerfeld's direct engagement with the empirical data—and especially his arguments in favor of particular empirical rules drawn from this data—far more problematic. Otto Klein described Bohr's reaction to Sommerfeld's *Zahlenmysterium* lecture in Lund as follows:

> During Sommerfeld's lecture I was sitting at the side of Bohr. Sommerfeld had a few numbers for these anomalous levels. The first was so and the second was so—they were something like 1, 3, and so. And then Sommerfeld said the next must be 5, or something like that. Then Bohr smiled and said to me, "I don't believe that."[96]

If it can be assumed that Landé was proceeding in a Sommerfeldian manner when he arrived in Frankfurt after working in Munich, Born's reaction must be adjudged far more extreme than Bohr's. Born largely ignored Landé, whose way of relating the intensities of multiplet lines and Zeeman effect lines through whole number ratios he could only describe as "horrible," in its obsessive "guessing about numerical values."[97] According to Robert Friedman, Carl Oseen's distaste for Sommerfeld's methods of research was, in large measure, responsible for Sommerfeld's failure to be awarded the Nobel Prize for physics in 1924, in spite of the enormous number of nominations he had received.[98]

Sommerfeld thus had good reasons for trying to establish his method as both subtle and coherent, neither number crunching nor numerology. And it is as an attempt to pitch the method precisely between these two extremes—emphasizing both the hard work involved in the technique and the knowledge and imagination required in its application—that we should read the following lines from the third edition of *Atombau*, perhaps the single clearest statement of the detailed practices in which Sommerfeld was engaged:

> It must not be imagined that the combination of the lines into series and their resolution into two terms is a mere trifle. Rather it demands special experience and ingenuity. First of all, the lines of the various series are all mixed together and must be separated out in accordance with the criteria indicated at the beginning of this section. There are usually only a moderate number of lines of a single series present, as the higher members of the series, on account of their feeble intensity, are less accurate than the more intense lower members. To derive the series limit and hence the constant first term of the series by extrapolation, the analytical expression for the current term, for example in the Ritz form, must be used as a basis. The series limit is then obtained, as well as the indeterminate parameters that occur in the series law…by a graphical or arithmetical process of approximation. It almost always appears that the first member (or members) of the series is not given with sufficient accuracy. From this we must conclude that

> not only Rydberg's but also Ritz's form represent only an approximation to the strict series law and are true only for the greater values of *m*.... The task of calculating the series becomes much easier if other series or series limits of the same element are already known. On account of the relationships of "combination"... between the different series, we have always to strike a balance between the calculations of several series.[99]

This, then, provides an understanding of a method that might be described as simultaneously a craft of the quantum and an investigation of number mysteries: A craft, in that, working directly with the data one extrapolates and interpolates, drawing conclusions not from model-based deductions, but from arithmetic and graphical approximations, drawing on special experience to strike a balance between different sets of the always-insufficient information from spectroscopic data. Finding that balance, however, and identifying the "correct" regularity in a sea of possibilities requires art and ingenuity, an inbuilt sense of the aesthetic, of the harmony that must rule within the atom. It was this second aspect—a rejection of the instrumentalist implications of what Forman has termed an *a posteriori* method—that Sommerfeld would emphasize in speaking of the values of mysticism in 1925.[100] "Precisely the most successful researchers in the area of theoretical spectral analysis, Balmer, Rydberg, Ritz, were genuine number mystics. They based their research, either consciously or unconsciously, on the claim that the connections of the wave numbers to spectra would have to be so harmonious, so aesthetically simple as to be compliant with the facts; and success justified their standpoint."[101] Conventionalism and positivism, he argued "sink into a nothingness before the beauty and security of our newest physical conclusions."[102] His was phenomenological practice fused with metaphysical belief, the robustness of empirical laws, gleaned with the aid of a delicate sense of aesthetics. Sommerfeld's was a music of the spheres composed by a craftsman: a beauty and a truth to be calculated and constructed, analyzed and approximated.

From the Old World of Waves to the New World of Quanta

In discussing Sommerfeld's postwar work on quantum spectroscopy, I have focused on detailing what his methodology was, or at least what it was meant to be. Just as important, however, is the question of what it was not. Throughout his papers and his texts, Sommerfeld sought time and again to distinguish his approach from that of Bohr. Even in 1919, Sommerfeld had been troubled by the implications of what he termed Bohr's "analogy principle" (labeled the "correspondence principle" soon thereafter). And in general, one can characterize the early 1920s for Sommerfeld as a period in which he drew away from the use of particular forms of analogical thinking in the atomic theory. Eschewing both mechanical models as analogies and the specific classical/quantum analogy that the correspondence principle denoted, in 1922 Sommerfeld turned instead to the "direct" empirical method we have discussed. The aim,

Conclusion

I was always satisfied if I could explain a certain complex of facts mathematically, without troubling myself too much with the fact that there were other things that didn't fit. Einstein, who always looks at the whole picture [*auf's Ganze blickt*], makes life more difficult for himself.

—A. Sommerfeld to J. Sommerfeld, December 24, 1928[1]

By the middle of 1925, Wolfgang Pauli was in a better mood than he had been in for some time. Only two months earlier, his exasperation with the state of theoretical physics had boiled over into a fit of pique. At the moment, his discipline, he acknowledged to Ralph Kronig in May, was developing apace; "nevertheless, it is much too difficult for me and I wish that I were a film-comedian or something similar and had never heard anything of physics!"[2] A letter written to Hendrik Kramers at the end of July revealed both his changed perspective and the personal reasons for his earlier dismay: "I feel at the moment a little less lonely as about half a year ago, when I found myself (spiritually as well as spatially) pretty much alone between the Scylla of the number mysticism of the Munich school and the Charybdis of the reactionary Copenhagen putsch propagated by you with the excesses of a zealot!"[3]

The timing of Pauli's last comment is significant. Six months before the letter to Kramers he had, in fact, produced the work for which he remains most famous and for which he received the Nobel Prize in 1945: the exclusion principle. Worked through at the end of 1924 and received by the *Zeitschrift für Physik* on January 16 of the new year, "On the Connection of the Closing of Electron Groups in the Atom to the Complex-Structure of Spectra" laid out Pauli's new quantum rule in simple, declarative terms: "There can never be two or more equivalent electrons in an atom for which, in strong fields, the values of all quantum numbers... coincide. If an electron is to be found in an atom for which these quantum numbers (in an external field) possess determinate values, then this state is 'occupied.'"[4]

As we saw in chapter 7, Pauli's sense that there were two main elements running through his work in the 1920s would remain with him. Shorn of its characteristic sarcasm, his sense of the significance of both the Sommerfeld and Bohr schools to his work on the exclusion principle reappeared in his Nobel speech.[5] Yet, although a considerable amount of space within a growing secondary literature on the history of quantum mechanics has been devoted to the importance to Pauli of the "Copenhagen putsch," almost nothing has been written on the corresponding significance of the Sommerfeld School's "number mysticism."[6] The point is even more striking for the absence of any mention of Sommerfeld in the development of quantum mechanics more generally. Although acknowledged as one of the most prolific and important contributors to the older quantum theory, not a single paper by Munich's professor of theoretical physics is to be found in B. L. van der Waerden's *Sources of Quantum Mechanics*.[7] Daniel Serwer's 1977 paper on Pauli and Heisenberg's reactions to the "unmechanical force" [*unmechanischer Zwang*] introduced by Bohr in the early 1920s excluded from the outset Sommerfeld's role in the further development of his former students' thinking in the crucial period 1923–1925. Insisting that his particular interest was in the *differences* between the two young men, Serwer avoided any extensive discussion of the ongoing impact of the similarities in their training:

> Sommerfeld was important for the basic education he offered Pauli and Heisenberg in the details of atomic spectra and in the use of the quantum-theoretical tools available to "save the phenomena." Since I assume Pauli and Heisenberg to have this basic education by 1923, I shall not have much to say about Sommerfeld. After they left Munich, Pauli and Heisenberg became increasingly concerned with whether the quantum mechanical postulates were adequate.[8]

Bohr's work, Serwer continued without further elaboration on what would appear to be the crucial point, "was more directly relevant to this concern than Sommerfeld's during 1923 to 1925."[9] Most recently, in a detailed study of the work leading up to the paper by Heisenberg that would launch the new mechanics, Michel Janssen and Anthony Duncan have argued that the problems central to the Sommerfeld School in the early 1920s were not only not useful to Heisenberg, but were actively obfuscatory: "...many of the other preoccupations of the old quantum theory, such as the detailed understanding of spectral lines, the Zeeman and Stark effects, and the extension of the Bohr-Sommerfeld model to multi-electron atoms (in particular helium), mostly added to the overall confusion and did little to stimulate the shift to the new mode of thinking exemplified by the *Umdeutung* paper."[10]

The aim of this concluding chapter is to delineate the ongoing historical and historiographical payoffs for the history of physics (and the history of science more generally) of the detailed study of Sommerfeld's "practice of theory." It proceeds in two parts. The first section takes the case of Pauli's path to the exclusion principle as a means of drawing out the importance of Sommerfeld's work—and that of his school—to the origins of the exclusion principle and to the birth of quantum mechanics. Accepting Janssen and Duncan's claim that the problems of spectroscopy were less significant to Heisenberg's *Umdeutung* than the more central dispersion problem, it is nonetheless argued that at the level of *method*, rather than of content alone, Sommerfeld's phenomenological turn in the 1920s was one element crucial to the development of the *discourse* of the new physics: its exclusive focus on "observable" quantities. The second section examines the reception within Sommerfeld's Munich school of Heisenberg, Born, and Pascual Jordan's matrix mechanics on the one hand, and Schrödinger's wave mechanics on the other. Schrödinger's approach, while acknowledged in many quarters to be less rigorous in conceptual terms, was lauded by Sommerfeld for its simple and powerful problem-solving capacities. Based as it was on familiar mathematical techniques, wave mechanics was almost tailor made for a physics of problems. In spite of its power and successes, however, Sommerfeld did not join many of his contemporaries (nor most subsequent analysts) in celebrating a new quantum-mechanical revolution. Indeed, as we shall see, his insistence that the new approaches constituted improvements but not ruptures in physical thought offers a deep insight into the connection between practice and participatory understandings of the nature of scientific change.

Exclusion

Magic, Harmony, and the Exclusion Principle

Pauli's path to the exclusion principle proceeded by way of two topics dear to Sommerfeld's heart: the anomalous Zeeman effect and the problems of *Atombau* and Röntgen spectroscopy.[11] Indeed, as the title of his paper suggests, the union of the solution to these apparently distinct problems provided the key to his success. He took up the anomalous Zeeman effect in late 1922, together with Bohr, who had agreed to write a short paper on the topic for a special issue of the *Annalen der Physik*, due in January 1923, celebrating the 70th birthday of the experimentalist Walther Kayser. The fact that Bohr did not send the article off until March led Pauli to quip that his mentor had effectively made Kayser younger by several months. Pauli himself was still stumped in June, writing to Sommerfeld with evident exasperation that it "would not, but would not come out."[12]

The problem with which Pauli was grappling was his attempt to explain the *Gesetzmässigkeiten* determined previously by Alfred Landé, like Pauli himself a former Sommerfeld student. In the early 1920s, Landé had incorporated and redefined the "inner" quantum number, j, to obtain a value for the size of line splittings in a weak magnetic field. Classically, such a field, when applied to a system like Bohr's planetary model of the atom, should cause all electrons to precess together at a given frequency around the field axis. The induced separations between given lines should then be proportional to this precessional (Larmor) frequency (i.e., $\Delta E = m\omega h$, with m integral). In the quantum case, however, Landé determined (empirically, after the fashion of Sommerfeld's *a posteriori* method) that the energy separation was given by the classical value multiplied by another term, the so-called *g*-factor (i.e., $\Delta E = g \cdot m\omega h$).[13] In 1921, when Landé first introduced this term, he could offer no physical interpretation of its meaning, other than that it was related to *j*, now understood as the total angular momentum of the atom.

A *modellmässig* explication of the *g*-factor had to await Heisenberg's publication, in 1922, of his *Rumpf* model of the atom. Infamously introducing half-integral quantum numbers, Heisenberg suggested that the observed splitting could be explained by the existence of a "coupling" between the angular momentum of a single, outermost electron (governed by *k*, the azimuthal quantum number) and the sum of the angular momenta of the remaining electrons (given by *r*), which formed the atomic core [*Rumpf*]. The sum of these two net momenta then gave, according to Landé, the total angular momentum of the atomic system, *j*. Doublets, in Heisenberg's peculiar vision, arose from a "sharing" of angular momenta: in effect, the outer electron gave a half quantum's worth of momentum to the core. This *ad hoc* move gave the right number of lines, but did so at the expense of any customary physical understanding.[14] In 1923, leaving most of the model's difficulties to one side, Landé deployed a conception similar to Heisenberg's to offer an expression for g[15]:

$$g = \frac{3}{2} + \frac{1}{2} \cdot \frac{R^2 - K^2}{J^2 - \frac{1}{4}}.$$

Pauli wrestled for months to provide, as he put it in a letter to Landé, "a satisfactory *modellmässige* meaning for such astoundingly simple *Gesetzmässigkeiten*."[16] His efforts were not crowned with success. When he published on the topic in April, he did so, he wrote to Sommerfeld, "with a tear in the corner of my eye," deeply unimpressed with what he had achieved.[17] Instead of *explaining* a peculiarity of the *Rumpf* model—the fact that the magnetism of the core appeared to be twice that which one would calculate from classical electron theory, while the magnetic moment of the external electron conformed to the classical result—Pauli proceeded "purely phenomenologically."[18] The odd doubling of the core's magnetic moment was, in effect, simply taken as an empirical datum.[19]

Heisenberg lauded the result, but Pauli had clearly had enough. For a year he withdrew from work on atomic physics, returning to the field only after accepting a brief to complete an encyclopedia article on the principles of the quantum theory in mid 1924. By the time he did so, his attitude toward the importance of modeling in quantum theory had undergone a radical transformation. As we saw in chapter 7, Pauli's highest praise for the fourth edition of *Atombau* (completed in October 1924) was reserved for its avoidance of *modellmässig* explanation for the problems of complex structure. A severe blow to a model-based method, however, had already been struck by Born and Heisenberg in early 1923. Taking up the problem of the helium atom, the two men demonstrated that, for the excited atom, detailed calculations using perturbation theory gave results irreconcilable with experiment. The failure of the Bohr-Sommerfeld model could no longer be attributed to insufficiently precise analysis. Pauli's negative reaction to the "reactionary Copenhagen putsch" and its faith in the powers of the correspondence principle had reached its zenith with the joint publication of a treatment of the dispersion problem using "virtual" oscillators and violations of the energy principle by Bohr, Kramers, and the Englishman John Slater. "I would always much rather say," he wrote to Kronig in 1925 with regard to the so-called BKS theory, "that I have so far no complete picture of the phenomena, than even temporarily to put up with a hideousness of this kind which hurts my physical sensibility."[20] Sommerfeld's number-mystical method no doubt appeared more appealing to Pauli as the reputation of its alternative seemed ever more tarnished.

In the midst of writing his encyclopedia article, Pauli hit upon a novel idea: a means of testing a fundamental assumption of the *Rumpf* model. If an alkali core had a non-zero magnetic moment (as it must when sharing some of the magnetism of the external electron), then g should depend on Z, the atomic number. Landé, tapped for data on the topic, soon returned the results: no dependence on Z, therefore no magnetic moment for a closed shell. The "sharing" model was dead. The cause of the anomalous Zeeman effect was not to be found in a peculiar coupling of the *Rumpf* with an external electron, but in some peculiar property of the electron alone. "The doublet structure of the alkali spectrum, as well as the violation of Larmor's theorem comes about through a peculiar, classically non-describable kind of *Zweideutigkeit* [ambiguity, doubled signification] of the quantum-theoretical characteristics of the light-electron."[21]

In a stroke, Pauli had solved (or, rather, dissolved) the problem of the *modellmässig* understanding of j and the cause of the apparent doubling of the magnetism of the atomic core. The *Rumpf* ceased to play any role in the production of spectral lines and hence the notion of a "total" angular momentum ceased to have any great significance. Since the violation of Larmor's theorem—the fact that g was not equal to unity—was the result of a "classically non-describable" characteristic of the outer electron, no model-based understanding should (or could) be sought. The *Zweideutigkeit* was a quantum property with no classical counterpart.

The "exclusion principle" proper was predicated on the notion that electronic behavior (and only that of electrons) was governed by four quantum numbers. The problem that it solved, however, arose not from the complexities of the Zeeman effect, but rather from the attempt to explain the processes of *Atombau* and the reason for the periodic structure of the table of elements. That question had been in Bohr's mind since his first quantum paper in 1913. It was not until his "second atomic theory," however, that he could develop what appeared to be a complete solution.[22] The theory was first revealed to the world in a letter to *Nature* in 1921, the same letter that, according to Sommerfeld, "battered in like a bomb," causing seismic shifts in his and his school's understanding of the processes of atom-building.[23] Two novel elements—together with the all-powerful correspondence principle—formed the essence of Bohr's second theory: the notion of "penetrating orbits" and the "construction principle" [*Aufbauprinzip*]. The first made explicit and detailed use of the Bohr model and argued that outer electrons in elliptical orbits about the atomic nucleus must penetrate the orbits of internal electrons, causing deviations in the Coulombic force acting upon them. Where, for Sommerfeld, the fact that the *Ellipsenverein* for the L shell intersected the circular K shell was an argument against the harmonious interlocking of electronic orbits, for Bohr the coupling between penetrating and inner electrons was essential to the theory.

Bohr's arguments proceeded by way of both analogy and disanalogy with the Bohr-Sommerfeld model of the Hydrogen atom. Characterizing each orbit by two quantum numbers, n and k ($n = 1, 2, 3, \ldots, \infty$; $k = 1, 2, 3, \ldots, n$), Bohr took up the question of the shape and size of each n_k orbit for elements with $Z > 1$. As was known from Sommerfeld's work on hydrogenic atoms in 1915, when $n = k$, orbits are circular; elliptical with increasing eccentricity as $n - k$ increases. The area enclosed by each orbit increases with n, so that any 4_k orbit, for example, is larger than any 3_k orbit. It is precisely this aspect that would change in Bohr's second theory. (See figure C.1.)

The notion that electrons "filled" lower orbitals in a fashion that reproduced the structure of the periodic table (two electrons in the lowest orbital, eight in the next, and so on) was one common to almost all models of atomic structure after Bohr's

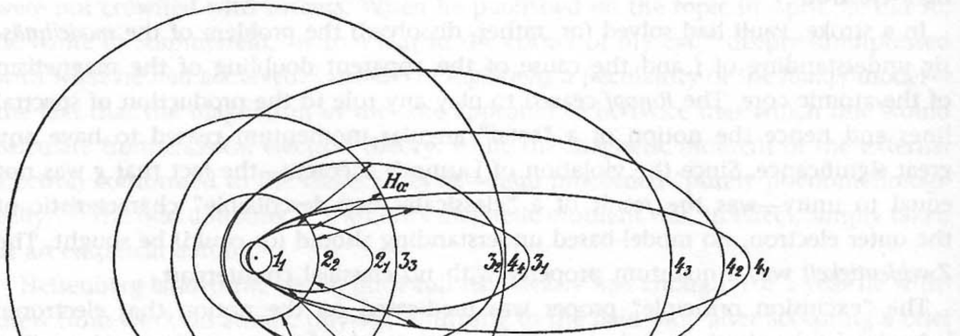


Figure C.1
Hydrogen orbits. Source: Niels Bohr, "The Structure of the Atom (Nobel Lecture, delivered December 11, 1922)," *Nature* (1923): 10.

first model in 1913. This implied, of course, that outer electrons in elements of higher atomic number than helium were "shielded" from the full nuclear force experienced by inner electrons. According to Bohr's analysis in the 1920s, however, some orbits for $n \geq 3$ penetrated lower orbitals. "Even though a 3_2 orbit will not penetrate into the innermost configuration of 1_1 orbits," he wrote in 1921 in a paper titled "The Structure of the Atom and the Physical and Chemical Properties of the Elements," "it will penetrate to distances from the nucleus which are considerably less than the radii of the circular 2_2 orbits."[24] In doing so, a 3_2 electron would feel the same force upon it—for this part of its orbit—as an electron in a lower orbital.[25] The effect would be to radically change the size and shape of its trajectory around the nucleus, shifting some elliptical orbits to lower overall energy states and causing the electron to trace out the shape of a rosary, rather than a single, repeated ellipse. Given that, as figure C.2 indicates, 4_1 and 4_2 orbitals are—contrary to the model of the Hydrogen atom—energetically more stable than 3_3 orbitals, one would expect these to be filled first. And so Bohr argued, at least for the first and second elements of the third period of the periodic table. After that, Bohr claimed that a "simple calculation" demonstrated that the increasing nuclear charge caused the higher 4_1 and 4_2 orbitals to increase in size in relation to a 3_3 orbit.[26] Electrons added to the structure of elements following Calcium ($Z = 20$) thus ceased filling the 4_1 orbits and began filling the 3_3 instead. Since the *Aufbauprinzip* held that the electronic structure of elements with $Z = N + 1$ was identical to that for element $Z = N$ except for the placement of the $N + 1$th electron, one could now explain the puzzling chemical

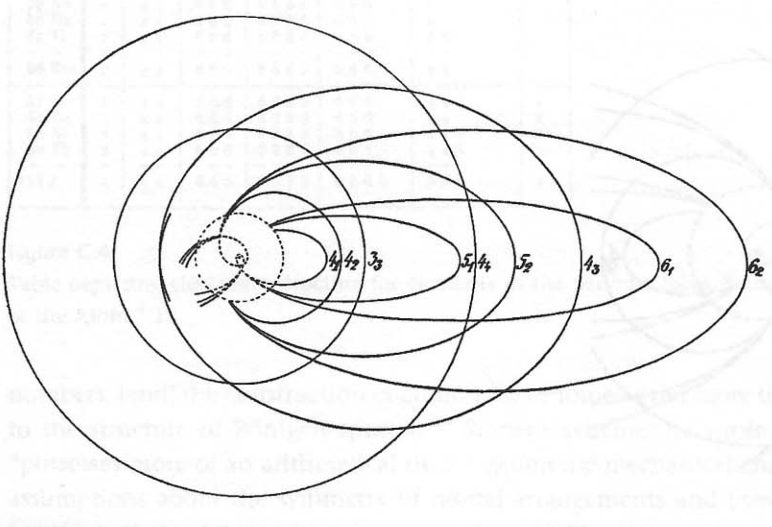


Figure C.2
Orbits of multi-electronic atoms. Source: Bohr, "Structure of the Atom," 12.

properties of the transition metals—and especially the "Lanthanides" and "Actinides"—in the table of elements. The elements from lanthanum ($Z = 57$) to lutetium ($Z = 71$) are, in spite of their increasing atomic numbers, chemically near-identical. In Bohr's theory, this followed from the fact that each such element possessed an identical number of *valence* electrons in a 6_1 orbital, even as each added more electrons to a previously empty (because previously higher energy) 4_4 orbit. Less convincing were Bohr's explanations of the *periodicity* of the periodic table. Why, for example, were there eight (and only eight) electrons in the second shell? For this, Bohr could only invoke somewhat vague symmetry arguments, which few outside Copenhagen seemed to find believable.[27]

Sommerfeld, originally enthusiastic about Bohr's seemingly miraculous calculations, soon became disillusioned as he and others in Germany realized that Bohr's results did not follow from detailed mathematical analysis at all.[28] Instead, even after being pressed for his method, Bohr could only invoke the power of the correspondence principle and his own intuition. The fourth edition of *Atombau* and a number of subsequent papers, as we have already seen, contained several explicit rebukes concerning Bohr's approach to the problems of atomic structure and reaffirmed Sommerfeld's distrust of *modellmässig* accounts. Much more promising seemed to be a new direction proposed by an English researcher, E. C. Stoner, in the *Philosophical Magazine* in October 1924. "According to Stoner," Sommerfeld wrote in his preface, dated the same month, "the shells in the interior of the atom are to be further subdivided, the number of electrons in the subgroups of the atomic shells are to be differentiated among themselves and are determined through the formal rules of the inner quantum

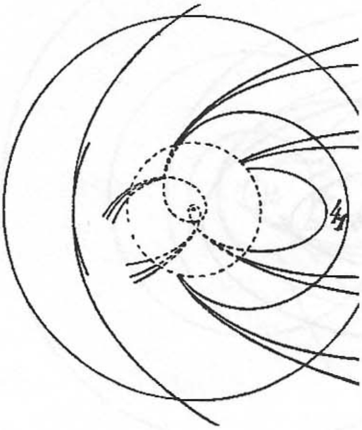
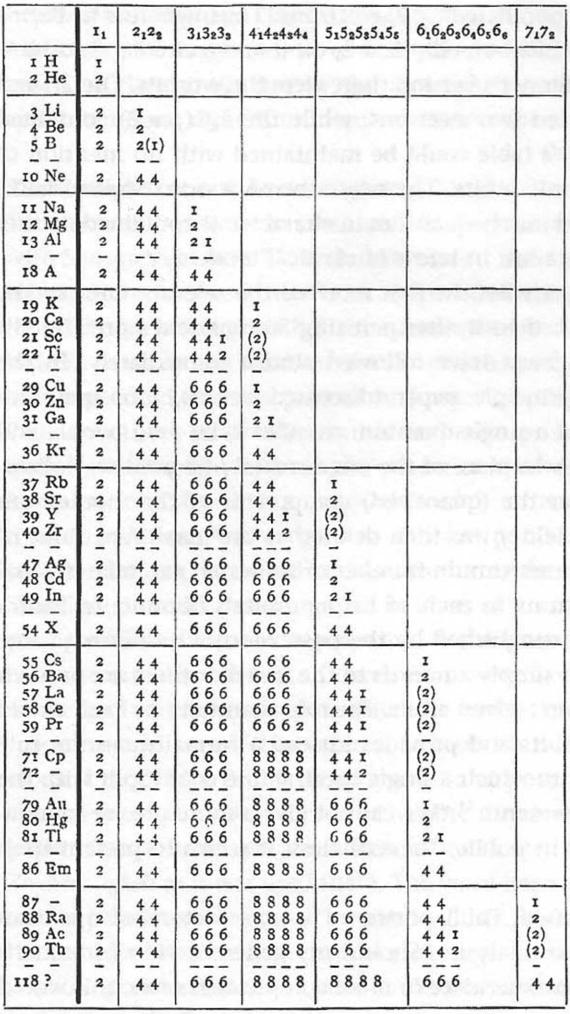


Figure C.3
Changed orbital shapes as electrons penetrate lower shells (section of figure C.2). Source: Bohr, "Structure of the Atom," 12.



	1_1	$2_1 2_2$	$3_1 3_2 3_3$	$4_1 4_2 4_3 4_4$	$5_1 5_2 5_3 5_4 5_5$	$6_1 6_2 6_3 6_4 6_5 6_6$	$7_1 7_2$
1 H	1						
2 He	2						
3 Li	2	1					
4 Be	2	2					
5 B	2	2(1)					
– –	–	– –					
10 Ne	2	4 4					
11 Na	2	4 4	1				
12 Mg	2	4 4	2				
13 Al	2	4 4	2 1				
– –	–	– –	– –				
18 A	2	4 4	4 4				
19 K	2	4 4	4 4	1			
20 Ca	2	4 4	4 4	2			
21 Sc	2	4 4	4 4 1	(2)			
22 Ti	2	4 4	4 4 2	(2)			
– –	–	– –	– – –	–			
29 Cu	2	4 4	6 6 6	1			
30 Zn	2	4 4	6 6 6	2			
31 Ga	2	4 4	6 6 6	2 1			
– –	–	– –	– – –	– –			
36 Kr	2	4 4	6 6 6	4 4			
37 Rb	2	4 4	6 6 6	4 4	1		
38 Sr	2	4 4	6 6 6	4 4	2		
39 Y	2	4 4	6 6 6	4 4 1	(2)		
40 Zr	2	4 4	6 6 6	4 4 2	(2)		
– –	–	– –	– – –	– – –	–		
47 Ag	2	4 4	6 6 6	6 6 6	1		
48 Cd	2	4 4	6 6 6	6 6 6	2		
49 In	2	4 4	6 6 6	6 6 6	2 1		
– –	–	– –	– – –	– – –	– –		
54 X	2	4 4	6 6 6	6 6 6	4 4		
55 Cs	2	4 4	6 6 6	6 6 6	4 4	1	
56 Ba	2	4 4	6 6 6	6 6 6	4 4	2	
57 La	2	4 4	6 6 6	6 6 6	4 4 1	(2)	
58 Ce	2	4 4	6 6 6	6 6 6 1	4 4 1	(2)	
59 Pr	2	4 4	6 6 6	6 6 6 2	4 4 1	(2)	
– –	–	– –	– – –	– – – –	– – –	–	
71 Cp	2	4 4	6 6 6	8 8 8 8	4 4 1	(2)	
72 –	2	4 4	6 6 6	8 8 8 8	4 4 2	(2)	
– –	–	– –	– – –	– – – –	– – –	–	
79 Au	2	4 4	6 6 6	8 8 8 8	6 6 6	1	
80 Hg	2	4 4	6 6 6	8 8 8 8	6 6 6	2	
81 Tl	2	4 4	6 6 6	8 8 8 8	6 6 6	2 1	
– –	–	– –	– – –	– – – –	– – –	– –	
86 Em	2	4 4	6 6 6	8 8 8 8	6 6 6	4 4	
87 –	2	4 4	6 6 6	8 8 8 8	6 6 6	4 4	1
88 Ra	2	4 4	6 6 6	8 8 8 8	6 6 6	4 4	2
89 Ac	2	4 4	6 6 6	8 8 8 8	6 6 6	4 4 1	(2)
90 Th	2	4 4	6 6 6	8 8 8 8	6 6 6	4 4 2	(2)
– –	–	– –	– – –	– – – –	– – –	– – –	–
118 ?	2	4 4	6 6 6	8 8 8 8	8 8 8 8	6 6 6	4 4

Figure C.4

Table depicting electronic structure for elements of the periodic table. Source: Bohr, "Structure of the Atom," 12.

numbers, [and] the construction of atoms is to be joined even more tightly than before to the structure of Röntgen spectra."[29] Stoner's scheme, he wrote soon afterwards, "possesses more of an arithmetical than a geometric-mechanical character, makes no assumptions about the symmetry of orbital arrangements and uses not only a part, but the entirety of Röntgen-spectroscopic facts."[30] This last point was essential. Further subdividing Bohr's n_k orbitals, Stoner used an extra quantum number, j, and spoke of

n_{kj} orbits.[31] Each such n_{kj} orbit was populated by $2j$ electrons. Thus, whereas in Bohr's conception there were two $n = 2$ orbits—an elliptical 2_1 orbit and a circular 2_2 orbit—each containing four electrons, in Stoner's version there were three orbits. The 2_{11} and 2_{21} ($j = 1$) subgroups each contained two electrons, while the 2_{22} ($j = 2$) contained four. The periodicity of Mendeleev's table could be maintained with no mention of the dynamical character of electronic orbits. The new scheme was, to Sommerfeld's satisfaction, formal, arithmetic, and purely quantum in character: it contained neither argument nor conceptual representation in terms of classical models.

Having passed over Stoner's paper when he first received the relevant copy of the *Philosophical Magazine*, Pauli returned to it after perusing Sommerfeld's preface. His "generalization" of Stoner's ideas must have followed almost immediately. In the notation used in his exclusion principle paper (discussed below), four quantum numbers were necessary. Instead of a single quantum number k, he used two: k_1 and k_2 ($k_1 = 1, 2, 3, \ldots, n$; $k_2 = k_1, k_1 - 1$). In place of the once-crucial j he used m_1, following Sommerfeld in defining this as the (quantized) component of the momentum parallel to an externally imposed field. j was then defined as the maximum value of m_1, given by $j = k_2 - \frac{1}{2}$. Clearly, the maximum number of values m_1 can take is equal to $2k_2$.[32] Stoner's $2j$ identical electrons in each of his n_{kj} orbitals become, in Pauli's formulation, $2k_2$ electrons, each distinguished by the possession of a different value of m_1. The exclusion principle then simply amounts to the fact that there are no such things as equivalent electrons within a given atom. The rule abandons, as Pauli would emphasize to Bohr, any talk of orbits and provides instead a formal quantum rule connecting the number of terms into which a single spectral line could split with the periodic structure of the table of elements.[33] "We cannot give a more precise foundation for this rule," he emphasized in public, "nevertheless, it seems to present itself very naturally."[34]

Reporting his result to Sommerfeld, Pauli portrayed it as a victory of quantum *Gesetzmässigkeiten* over model-based analysis. "Should my generalization of Stoner's ideas also, in the future, stand up to experience in more complicated cases, this would then simultaneously signify that you were completely right as regards the problem of the closing of electronic groups within the atom 'to place greater hope in the magic [*Zauberkraft*] of quanta than in correspondence- or stability-considerations.'" I do not, in fact, believe, he continued, "that the correspondence principle has anything to do with this problem."[35] Sommerfeld, studying the published version for one of his lectures, declared it "very beautiful and doubtless correct."[36] Bohr was equally impressed, but resisted Pauli's conclusion that his result signified the death of the correspondence principle. Even he, however, noted the elements of Sommerfeldian number-mysticism—the magic of quanta—in Pauli's paper. "I am also not entirely sure whether you do not step over a dangerous line if you—as you intone your old 'Carthage must be destroyed'—pronounce the final death sentence of a correspondence-based explanation of group closure." Pauli's own "lovely number-harmonies" [*smukke Talharmonier*], he suggested, were not entirely free from "poor, classical conceptions of space," a claim intimated by the fact that there was one quantum number for each spatio-temporal dimension required to describe an electronic trajectory.[37]

Zweideutigkeit about *Zweideutigkeit*

The discussion thus far has centered on the years after Pauli completed his dissertation with Sommerfeld in 1921. It should be clear that it is impossible to ignore the ongoing intersections between their work. Although Pauli took up the problem of the anomalous Zeeman effect with Bohr's encouragement, his approach to its many puzzles—indeed, in many ways the very framing of the problem itself—was molded by the work of Sommerfeld and his present or former pupils, including Heisenberg and Landé. Pauli's method, in developing his exclusion principle, was similarly Sommerfeldian both in its skepticism about the power of a *korrespondenzmässig* approach and in its focus on formal quantum rules gleaned from empirical data, with little analysis of their foundation. With regard to this last point, it is worth emphasizing that Pauli (and Heisenberg) were both at Munich during the precise period in which Sommerfeld abandoned model-based analysis in favor of his harmonious lawful regularities. Both young men participated in preparing the volumes of *Atombau* that recorded the shift in Sommerfeld's thinking. Indeed, Pauli would note in 1924 that the fourth edition of the text was the first upon which he had not worked.[38]

Sommerfeld's work thus offered, as Pauli himself would suggest in 1945, a methodological model for Pauli's development and postulation of the exclusion principle. It also, as we shall now see, offered a more direct resource for the content of the 1925 paper. To see how, one must look more closely at the precise meaning of the term *Zweideutigkeit* as it was used there. The word has a customary meaning in German and can be translated simply as "ambiguity." In Copenhagen in the early 1920s, however, the term had acquired a technical meaning—"two-valuedness"—and signified the two possible positions that the core could take up under the action of Bohr's *unmechanischer Zwang*.[39] Pauli used the term to mean something similar to this in a letter to Landé in September 1923. Rewriting Landé's expression for g as

$$g=\frac{3}{2}+\frac{1}{2}\frac{r(r-1)-k(k-1)}{j(j-1)},$$

Pauli then pointed out that "each momentum will act not through a single number, but through a *pair* of numbers. The momenta appear in a certain sense to be *zweideutig*.... One sees further that this *Zweideutigkeit* also includes k."[40] *Zweideutigkeit* in this sense refers to the two values that a *single* quantum number can take. In understanding what Pauli meant by the term in 1925, van der Waerden has used essentially the same notion.[41] Acknowledging that Pauli's statements about the *Zweideutigkeit* in