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The historical role of the Adiabatic Principle in Bohr's quantum theory

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It is widely known that both the Correspondence Principle and the Adiabatic Principle were the two pillars of Bohr's quantum theory. However, the Correspondence Principle usually gets much more attention in historical accounts. A closer look at Bohr's quantum theory shows that, although the fate of the Adiabatic Principle was closely tied up with the validity of mechanics, it also played a significant role in the old quantum theory. In the early 1920s, when dealing with multielectron atoms, Bohr was forced to reshape the theory and thus to reconsider the relative relevance of the two principles. It is precisely the late preponderance of the Correspondence Principle which has, in perspective, biased the historical weight attributed to each of them.

The *old quantum theory* is considered to start with the appearance of the quantum hypothesis, in 1900, in Max Planck's hands. Despite its name, for two decades there was not any unique and well-defined theoretical framework. Instead, a fragmentary collection of semi-classical theories, models, and applications, accounted for most of the experimental results. With the gathering of more detailed, precise data and, especially, with the increasingly elaborate attempts of unification, the departure from classical conceptions was forced upon the conceptual foundations, ultimately giving rise to quantum mechanics in 1925 [1].

1 From hypothesis to principle

In 1911, Paul Ehrenfest used for the first time adiabatic invariants within the quantum framework [2]. Two years later, he announced what, after Einstein, later became known as the *adiabatic hypothesis*, which established the adiabatic invariants of a mechanical system as the quantities to be quantized [3]. After a few years in which it went essentially unnoticed, in 1916 Bohr embraced it in one of the first reformulations of his theory. He used for the first time adiabatic invariants to give it consistency, and more specifically to justify the selective application of mechanics [4]. However, Bohr withdrew the paper as a reaction to Sommerfeld's latest contributions, in order to update his theory [5]. Thus his use of Ehrenfest's hypothesis remained unknown for the time being.

In a letter to Sommerfeld in 1916, Ehrenfest congratulated Sommerfeld for the successes achieved in Munich, but he added that he found "appalling" that they "will help the provisional but still so cannibalistic Bohr model to obtain new triumphs." [6] Beyond doubt, Bohr's trilogy of 1913 had "plunged" him "into despair," even after he had checked the compatibility of his hypothesis with Bohr's atomic model [7]. However, Ehrenfest's disappointment with Bohr's ideas would not last for long: the two would soon get acquainted and develop a strong friendship which, at the same time, converted Ehrenfest into an enthusiastic proponent of Bohr and his quantum theory (figure 1).

By updating his theory, Bohr re-established the foundations from scratch, with a systematical approach to build a self-consistent theory starting only from a few principles [8]. If this paper was a reaction to Sommerfeld's breakthroughs of 1915 and 1916, in its turn it became highly inspirational for Sommerfeld's further developments on the theory, as shown by the subsequent editions of *Atombau und Spektrallinien* [9].

In 1918, Bohr based the theory only on two postulates—namely those that he had originally stated in 1913 and that have become famously associated to his name—and on one principle which rested on Ehrenfest's adiabatic hypothesis. We also notice the appearance

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Figure 1 Niels Bohr, Paul Ehrenfest and his son Pavlik Ehrenfest Jr. at the Leiden railway station, probably around 1925. Courtesy of the Niels Bohr Archive, Copenhagen.

of a precursor of the Correspondence Principle, which at this point Bohr still called only an "application" or "reasoning" instead of a "principle", and its role was clearly secondary. The main guarantor of the theoretical inner consistency was the so-called *Principle of Mechanical Transformability*—as Bohr had rebaptized the adiabatic hypothesis.

That Bohr's treatment of this issue stood out was clear at first sight: what for Ehrenfest used to be an unproved hypothesis, now became in the hands of the Dane a needless-to-prove *principle* upon which the theory itself rested. The adiabatic invariants were the quantities to be quantized, an undisputed claim because the stability and inner coherence of the theory itself depended on this principle. Furthermore, in the purely formal landscape, this principle allowed the establishment of the energy differences between electronic orbitals, removing an arbitrariness of previous versions of Bohr's theory. Also in a more pragmatical way, the Principle of Mechanical Transformability had important applications: it was used to connect known stationary states with *unknown* ones, simply via the (slow) addition of an external field. It was also used to establish rules concerning the statistical treatment of quantum systems, a result that Bohr had already foreseen in his 1916 paper but that in 1918 was developed in more detail (also thanks to the developments made by Ehrenfest's disciples Jan Burgers and Iurii A. Krutkow [10]).

Furthermore, Bohr extended the range of applicability of adiabatic transformations to degenerate systems, even for transformations which caused a change in the number of degrees of freedom; a problem of which Ehrenfest would later claim that he himself had "stood helpless before it." [11]

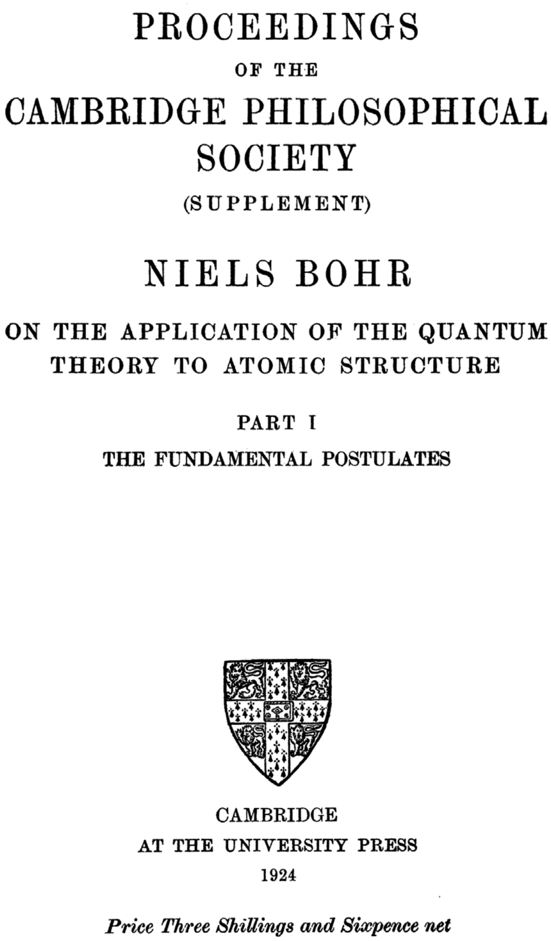
As we have said, there was no such thing as a "Correspondence Principle" in Bohr's 1918 theory; only a primitive version of its essence and some of its applications were present. By rights, one could even trace some aspects of the Correspondence Principle back to his initial trilogy of 1913. For example, the use of the large n limit to assess the convergence of the theory towards classical physics in the required cases. But it would not be until 1918 that some deductive applications of this principle would start to appear, mainly thanks to the contributions of Hendrik A. Kramers [12]. The Correspondence Principle itself would not make a full appearance in Bohr's words until 1920, in a meeting of the *Deutsche Physikalische Geselleschaft* in Berlin [13].

2 Reshaping of Bohr's theory: new roles, new principles

By 1920, Bohr could justify some properties of the periodic table of elements, a result that was considered a great feat of his theory. However, in order to fully expand the theory from hydrogen to the rest of elements, Bohr needed to widen its foundations and to account for much more complex systems: acknowledging that he could not explain complex atoms only with multiperiodic motions, he tried to take his theory one step further and overcome the limitations of mechanical periodic systems.

The main consequence of this shift from *multiperiodic* to *multi-electronic* was the overthrowing of mechanics. If complex atoms were to be explained with his quantum theory, this could never be with some mechanically compatible periodic equations. In this new phase of the theory—the fundamentals of which were finally written down by Bohr by the end of 1922, after a somewhat unproductive period related to overworking—, the organic relationship between mechanics, electrodynamics and the quantum principles reshaped into a new form [14]. What before used to be a theory built on the grounds of the validity of mechanics, now was usually referred to as resting on "ordinary electrodynamics." And this, only to be immediately dismissed as unable to account for the multielectron atoms.

In this change of vocabulary we glimpse a shift in Bohr's ideas. Despite the rejection of the old mechanics, for the hydrogen atom the theory had fared very well. By presenting the theory as a generalization of classical physics, Bohr saved these accomplishments while leaving the door open to further departures from classical conceptions. However, we believe that one of the



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NIELS BOHR

ON THE APPLICATION OF THE QUANTUM THEORY TO ATOMIC STRUCTURE

PART I
THE FUNDAMENTAL POSTULATES

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1924

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Figure 2 Cover of the English translation to Bohr's *Grundpostulate*, published in 1924 in a supplement to the *Proceedings of the Cambridge Philosophical Society* [14, p. 1].

main reasons why Bohr chose to change his written expression—from "mechanics" to "electrodynamics"—was an actual change in his regard for the principles: in 1922, there was already a Correspondence Principle with full rights of its own. This principle had become the precious gem of his theory really quickly, stepping over the Adiabatic Principle and finally overthrowing it from its privileged position—at least from a practical point of view.

We find proof of the growth of the role of the Correspondence Principle in the elaboration of the new treatise on the theoretical foundations—partially published in 1923 (figure 2). In this paper, Bohr brought the definition and presentation of the Correspondence Principle to the early pages of the fundamental postulates (*Grundpostulate*), giving it a much higher relevance than in previous publications. On the contrary, the role of the Adiabatic Principle seems much diminished: not only because it appears farther behind the Correspondence Principle, but especially because its applications are now scarce. Nevertheless, in Bohr's words, the Adiabatic Principle apparently retains a major role at the same level as the Correspondence Principle: [14, p. 42]

> [T]he Adiabatic Principle, as well as the Correspondence Principle, occupy a different position, because of their more general range of applicability. They appear, as we shall see, suited, in a higher degree, to point out new ways for further extensions of the quantum theory of atomic structure.

Despite these statements, from a practical point of view the Adiabatic Principle appears to be secondary for Bohr. Due to the extension of the theory beyond mechanical limits (or rather the limits of ordinary electrodynamics, as Bohr would put it), new principles are forged by Bohr to guarantee the inner consistency of the quantum theory, and they inevitably take over some roles previously assigned to the Adiabatic Principle.

Thus, a new principle is introduced by Bohr in order to guarantee the stability of quantum states: the *principle of existence and permanence of the quantum numbers*. Where the Adiabatic Principle used to guarantee such stability of the electron orbits, now Bohr simply stipulates it. In another range of applicability, but very related to this principle, we find the so-called *Aufbauprinzip*: it establishes certain rules for the process of building up of multielectron atoms, an unnecessary concern when the theory rested on mechanical assumptions. However, it is precisely because of the failure of mechanics that a new principle was needed in order to guarantee the correct behavior of atoms during their construction (*Aufbau*). Moreover, even if the Correspondence Principle rests upon electrodynamics, its limitations also needed to be tackled with the introduction of yet another principle: the *Coupling Principle*, which plays a role in the interactions between quantum systems—a phenomenon clearly departing from any possible explanation by mechanics or ordinary electrodynamics—by treating the system as a whole, in a manner similar to the proper modes in the black body radiation problem. These new principles were not much detailed at this early stage, but rather depicted by the general directions which, according to Bohr, the theory had to take in future developments. The Coupling Principle, for example, seems to be a prelude to the ideas of the unsuccessful BKS theory [15].

What is clear from these new principles is that the Adiabatic Principle was losing ground and its role was being taken over by other principles. Mostly the *principle* *of existence and permanence of the quantum numbers*, but also the Correspondence Principle took part in this usurpation: in 1922 Bohr attributes to the latter "a point of attack on the problem of the stability of the normal states of the atom, fundamental to the discussion of the properties of elements." [14, p. 25] In this quote we see how a role that was usually played by the Adiabatic Principle is now attributed to the Correspondence Principle. We cannot help but suspect that there is a link between the success in explaining the periodic table (what he called "the properties of elements") and this change of weight between the two most important principles in Bohr's theory. All in all, the Correspondence Principle had proven an almighty tool.

3 From the old quantum theory to quantum mechanics

The amendments Bohr introduced to the Adiabatic Principle after 1922 were motivated by the gradual breakdown of the old quantum theory itself. Multiple instances showed that the results were definitively incompatible with mechanical and electrodynamical conceptions, and the severe departure from these frameworks made the survival of the Adiabatic Principle in its original form impossible. Bohr still claimed its key relevance, but from a practical point of view he abandoned it: the Adiabatic Principle was becoming less and less adequate to fit in with the rest of the theoretical structure.

However, the applications of this hypothesis by other physicists in the early 1920s show that it was still valuable. There were adiabatic transformations performed in the construction of atomic models, and refinements of Burgers' demonstration of the adiabatic invariance of the quantum rules appeared as late as 1925 [16]. In the few existing monographs on the quantum theory previous to the appearance of quantum mechanics, the Adiabatic Principle was always presented as a crucial element to keep the consistency of the theory [17].

Bohr did not openly accept any criticism of the Adiabatic Principle until the results of crossed fields forced him to do so: the analysis of the simultaneous application of an electric and a magnetic field with an angle different from zero to a sample of hydrogen convinced him of the untenability of the Adiabatic Principle even in systems where mechanics was valid [15].

When quantum mechanics emerged, the Adiabatic Principle was quickly translated into the new language, but its new role was far from fundamental [18]. By contrast, the Correspondence Principle was seen as a key precursor of the dispersion theory by Kramers and of Heisenberg's *Umdeutung*. Bohr himself contributed to the inception of this narrative in the first publication in which he commented on the new approach [19]. It is probably because of that alleged continuity with the new mechanics that nowadays the Correspondence Principle receives much more attention in the historical accounts of the quantum theory than the Adiabatic Principle does.

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