Spinning Electrons on Pendulum-Paths in Hydrogen Atoms

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Abstract

While electronic orbitals with zero orbital angular momentum are a standard feature of modern quantum mechanics, the corresponding linear electron paths with zero orbital angular momentum ("pendulum-paths") were explicitly excluded in the "old quantum theory" because of concerns that an electron on such paths would collide with the atom's nucleus. Recently, Rivas hypothesized that his model of spinning electrons allows for electrons on pendulum-paths without collisions with the nucleus. In the present work, the scenario of a spinning electron in a hydrogen atom on a pendulum-path was numerically simulated using relativistic equations of motions by Beck. The resulting trajectories were evaluated by comparing time-averaged powers of the distance between electron and proton with corresponding time-averaged values in an improved variant of the Bohr-Sommerfeld model as well as with quantum mechanical expectation values. The numerical results for a spinning electron were in better agreement with quantum mechanical expectation values than the results for the improved Bohr-Sommerfeld model.

1 Introduction

While the Bohr-Sommerfeld model [Som23] predicted the fine-structure of energy levels of hydrogen-like atoms as accurately as Dirac's theory of the electron, it failed in many other cases. Some of these shortcomings were unavoidable considering that the original Bohr-Sommerfeld model treated electrons as spinless particles. Other shortcomings could have been avoided by relatively small amendments. This is especially true for the orbital angular momentum of electrons and the corresponding azimuthal quantum number l as discussed, for example, by Born and Jordan [BJ30], Pauling and Wilson [PW35], Pauling [Pau60], and Bucher [Buc08]. Specifically, it is preferable to choose values $l = 0, \ldots, n-1$ instead of $l = 1, \ldots, n$ (with the primary quantum number n) and to set the corresponding orbital angular momentum to $\hbar\sqrt{l(l-1)}$ instead of $\hbar l$ or $\hbar(l-1)$.

Bohr and Sommerfeld's actual reasons for their choice were probably rather complex as discussed in some detail in Section 2.2. However, the main reason that Bohr and Sommerfeld provided in their writings was the concern that an electron on an orbit with zero orbital angular momentum (i.e. a pendulum-path) would collide with the nucleus of the atom. Since then, researchers have been considering physical processes that would allow for pendulum-paths, e.g., elastic collisions [DL74], penetrations of finite-size nuclei [Buc06], or pendulum-paths as very narrow ellipses [Eps62]. However, none of these models has been particularly successful. Recently, Rivas hypothesized that a spinning electron on a pendulum-path avoids a collision with the nucleus by spiraling around it at a safe distance [Riv24]; see Section 2.1 for more details.

Unfortunately, Rivas did not provide any quantitative results for a spinning electron on a pendulum-path. Therefore, the main objective of the present work was to numerically simulate this scenario in an idealized hydrogen atom with an infinitely heavy proton. To this end, the equations of motion of Beck's model [Bec23] were implemented as described in Section 3. Additionally, a variant of Beck's model using half the spinning frequency and twice the spinning radius [Kra24] was implemented for comparison. The maximum distance of the simulated electron from the proton as well as the time period from perihelion to perihelion matched the expected values for pendulum-paths [DL74, Buc06] providing numerical evidence that Rivas' hypothesis is correct.

The simulated trajectories were further analyzed by numerically computing time-averaged values of r, r^2, $1/r$, and $1/r^2$ with r denoting the distance between electron and proton. This approach was motivated by Pauling and Wilson's comparison of analytic expressions for these values in an improved

Bohr-Sommerfeld model and corresponding quantum-mechanical expectation values [PW35]. Results are presented and discussed in Section 4. Conclusions and future work are presented in Section 5.

2 Previous Works

2.1 Models of Spinning Electrons

The models of spinning electrons that are relevant for the present work describe an electron as a point-like charge (at the "center of charge") that spins around a "spin center" (or "center of mass"). Examples include models by Rivas [Riv24], Beck [Bec23], and Kraus [Kra24]. A common feature of these models is that the electromagnetic Lorentz force on the electron is computed for the position of the point-like charge, but it accelerates the movement of the spin center, which, therefore, moves approximately like an electron with spin. The differences between the mentioned models of spinning electrons include, for example, radius and frequency of the spin motion around the spin center in the rest frame of the spin center.

Based on his model of spinning electrons, Rivas hypothesized: "In the ground state of the Hydrogen atom the electron is in [an] S-state of orbital angular momentum $l = 0$. This implies, from the classical point of view, that the center of mass of the electron is going through the center of mass of the proton. This is impossible for the spinless point particle. Nevertheless this can be justified classically, because the center of mass and the center of charge of [...] spinning electrons are different points and their separation is greater than the estimated size of the proton. Then in the ground state of the atom the center of mass of the electron describes a straight trajectory passing through the center of mass of the proton" [Riv24, page 18, prediction no. 39]. In other words, Rivas argues that in the ground state of a hydrogen atom, the center of mass of a spinning electron is on a pendulum-path without the center of charge colliding with the proton. The same hypothesis appears to apply to the models of spinning electrons by Beck [Bec23] and Kraus [Kra24]. The main distinguishing feature of the latter model [Kra24] is that it spins half as fast at twice the radius in comparison to Beck's and Rivas' models.

2.2 The Rocky History of Pendulum-Paths

Since electrons in the Bohr-Sommerfeld model of atoms [Som23] move on classical trajectories around an atom's nucleus, one might expect that an electron's state of zero orbital angular momentum is represented by a linear path straight through the nucleus, i.e., a pendulum-path ("Pendelbahn" in German). Historically, however, this is not how the Bohr-Sommerfeld model represented such states. Bucher argued that this feature (or "flaw") of the Bohr-Sommerfeld model accelerated its downfall and the rise of modern quantum mechanics [Buc08]. Therefore, this section tries to trace the history of this feature of the Bohr-Sommerfeld model in quite some detail. Readers who are only interested in more recent research on pendulum-paths (after 1920) are encouraged to skip forward to the last paragraph of this section.

What motivated Bohr and Sommerfeld to exclude pendulum-paths? Sommerfeld stated that "the electron, in describing this orbit would fall into the nucleus. Owing to the permanence of atoms we regard this as impossible" [Som23, page 238]. Similarly, Bohr stated that "for certain external fields such motions cannot be regarded as physical realisable stationary states of the atom, since in the course of the perturbations the electron would collide with the nucleus" [Boh18, page 56]. Were Bohr and Sommerfeld just too narrow minded to consider the possibility of pendulum-paths?

Interestingly, some of Bohr's earlier publications [Boh14, Boh15, Boh16] and at least one of Sommerfeld's publications [Som17] show that they had accepted the possibility of pendulum-paths just a few years earlier. And they were not alone: Epstein (who coined the term "Pendelbahn") was sure that they had been observed in experiments by Stark [Eps16, Eps19]; and even the grandfather of quantum physics, Max Planck, did not dismiss the idea [Pla20]. Thus, physicists at the time had been more than open to the idea of pendulum-paths. What else could have changed Bohr's and Sommerfeld's minds in the years around 1917?

In 1930, Born and Jordan described Bohr's and Sommerfeld's decision in this way: "In Bohr's theory—due to the quantum conditions for the orbital angular momentum quantum number, which was usually referred to as the azimuthal quantum number k—all values $k = 0, 1, 2, \ldots, n$ were initially permissible for a given n. [...] However, the number $n + 1$ of these values is 1 more than observed

in experiments. Therefore, the case $k = 0$ (which would have corresponded to a pendulum-path with the electron passing through the nucleus) was excluded by a special 'extra rule;' however, this gave rise to other difficulties"[1] [BJ30, pages 189–190]. (Some of these "other difficulties" were described in 1926 by Pauli [Pau26].) Thus, according to Born and Jordan, experimental results (specifically the number of spectral lines in observations of the Stark effect and the Zeeman effect) confronted Bohr and Sommerfeld with the choice of either excluding pendulum-paths or excluding circular orbits. Since it was unclear why pendulum-paths would not result in collisions with the nucleus, Bohr and Sommerfeld decided to introduce an extra rule that excluded pendulum-paths.

While this description by Born and Jordan is plausible, it cannot be the whole story: If Sommerfeld's primary objective had been to match the experimental results, then he would have had no reason to change his opinion about pendulum-paths after 1917 when he had accepted the possibility of pendulum-paths in observations of the Stark effect as described by Epstein, who wrote in 1916: "the electron oscillates in a straight line along the x-axis between two fixed points, coming infinitely close to the nucleus. Without an external electric field, such an orbit (a Keplerian ellipse of eccentricity 1) is impossible for relativistic-energetic reasons, which is why Sommerfeld does not consider it when calculating the doublets of spectral lines. However, observations of the Stark effect show that they undoubtedly occur here, even though the components associated with them are extremely weak"[2] [Eps16]. Sommerfeld appeared to agree with Epstein's statement in 1917 when he wrote: "when an electric field is applied, however, pendulum-paths appear to be able to occur with weak intensity"[3] [Som17]. A few years later, Epstein employed concepts of modern quantum mechanics to show that his explanation of the Stark effect from 1916 (confirmed in 1919 [Eps19]) was as good as possible within the framework of the Bohr-Sommerfeld model [Eps26]. Thus, whatever motivated Sommerfeld to change his opinion about pendulum-paths, it was neither supported by experimental observations of the Stark effect nor by modern quantum mechanics.

Is it possible that another expert on the Stark effect convinced Sommerfeld after 1917 to mistrust Epstein's explanation? At the time, the only serious alternative to Epstein's explanation of the Stark effect had been published by the famous Karl Schwarzschild [Sch16]. The story of how Sommerfeld caused Epstein and Schwarzschild to work on the Stark effect at the same time was recounted by Epstein in an interview in 1962 [Eps62]. Sommerfeld was well aware that Epstein reached the correct equation describing the Stark effect first, and that Schwarzschild had to revise his own article before publication. Nonetheless, if Schwarzschild had tried to convince Sommerfeld that Epstein was wrong about pendulum-paths, Sommerfeld might have trusted Schwarzschild's well-known expertise in celestial mechanics. However, it is very unlikely that it was Schwarzschild who changed Sommerfeld's opinion in 1917 or later, first of all because Schwarzschild had tragically died in May 1916.

Who else could have changed Sommerfeld's opinion? The quote by Born and Jordan includes another hint: the rule that excluded pendulum-paths [BIF34]. Epstein mentioned this extra rule in his 1926 publication and attributed it to Bohr without providing a source [Eps26]. Fortunately, Sommerfeld provided more details in the 2nd edition of his book „Atombau und Spektrallinien"[Som21]: "From a historical perspective, it should be noted that our discussion regarding the reality or unreality of the components deviates somewhat from Epstein's original one. We relied on our theoretically based selection principle together with Bohr's rule prohibiting vanishing azimuthal quantum numbers. Epstein, on the other hand, used a more empirical selection principle (previously advocated by the author but now abandoned)"[4] [Som21, pages 451–452]. Sommerfeld provided the source for Bohr's

[1] Original passage in German: „In der Bohrschen Theorie waren nämlich auf Grund der Quantenbedingungen für die Impulsquantenzahl, die gewöhnlich als ‚Nebenquantenzahl' k bezeichnet wurde, bei vorgegebenem n zunächst alle Werte $k = 0, 1, 2, \ldots, n$ zulässig. [...] Die Anzahl $n + 1$ dieser Werte ist aber gegenüber der experimentellen Erfahrung um 1 zu groß. Man hat deshalb den Fall $k = 0$ (der einer „Pendelbahn" mit Durchgang des Elektrons durch den Kern entsprochen hätte) durch ein besonderes "Zusatzverbot" ausgeschlossen; dabei ergaben sich jedoch anderweitige Schwierigkeiten." [BJ30, pages 189–190]

[2] Original passage in German: „[D]as Elektron pendelt in der x-Achse geradlinig zwischen zwei festen Punkten hin und her, wobei es dem Kern unendlich nahe kommt. Ohne ein äußeres elektrisches Feld ist eine solche Bahn (eine Keplerellipse von der Exzentrizität 1) aus relativistisch-energetischen Gründen unmöglich, weshalb sie auch Sommerfeld bei Berechnung der Dubletten von Spektrallinien nicht in Betracht zieht. Die Beobachtungen über den Starkeffekt zeigen aber, daß sie hier ohne jeden Zweifel auftreten, wenn auch die zu ihnen gehörenden Komponenten äußerst schwach sind" [Eps16].

[3] Original passage in German: „bei Anlegung eines elektrischen Feldes dagegen scheinen Pendelbahnen mit schwacher Intensität auftreten zu können" [Som17].

[4] Original passage in German: „In historischer Hinsicht sei noch bemerkt, daß unsere Diskussion bezüglich der Realität oder Irrealität der Komponenten von der ursprünglichen Epsteinschen etwas abweicht. Wir stützten uns auf unser

rule in a footnote on page 431, namely the 2nd part of Bohr's work "On the Quantum Theory of Line-spectra" [Boh18]. In the same footnote, Sommerfeld summarized Bohr's reason for this extra rule: the eventual collision of the electron with the nucleus.

It is probably worth repeating that even Planck was not too worried about the electron colliding with the nucleus [Pla20], and Sommerfeld appeared to have overcome his concerns by 1917 [Som17]. Epstein was asked in an interview [Eps62] whether "the problem of eventual collision in some of these orbits [was] considered to be a grave one." Epstein replied: "Not to my knowledge, except by mathematicians. You see, I remember that I talked about this point to Weyl, that is whether it makes sense to use such an orbit, and he thought no, it should be excluded. But we just kept it in" [Eps62]. The main reason for the extra rule excluding pendulum-paths that was provided by Bohr was the concern about an eventual collision with the nucleus, which had not stopped him in earlier publications [Boh14, Boh15, Boh16]. Thus, the issue of an eventual collision with the nucleus was probably not considered a compelling scientific reason (not even by Bohr and Sommerfeld) but a mechanical analogy to make plausible the exclusion of pendulum-paths. As mentioned by Born and Jordan, it also allowed Bohr and Sommerfeld to keep circular orbits in their model of hydrogen-like atoms without having to explain their reasons. For Sommerfeld, in particular, it was convenient to be able to refer to Bohr's extra rule [Boh18] when writing his book on atomic structure and spectral lines [Som21].

For Bohr, on the other hand, there was an event in early 1916 that might have contributed to his extra rule: Sommerfeld had sent him some early articles on the fine structure of spectral lines of the hydrogen atom, which caused Bohr to withdraw at least one planned publication [Eck13, page 213]. In Sommerfeld's articles [Som15b, Som15a], he excluded pendulum-paths based on concerns about collisions with the nucleus and infinite velocities [Som15b]. He also stated his strong intention to include circular orbits: "the circular orbit, which we will in any case declare to be possible"[5] [Som15b, page 445]. As mentioned, these reasons did not stop Sommerfeld from changing his mind about pendulum-paths in 1916 or 1917 [Som17]. However, they might have convinced Bohr to propose an extra rule in 1918 [Boh18], which then encouraged Sommerfeld to exclude pendulum-paths again in his book [Som21]. (Even some figures from earlier publications [Som16, Fig. 4 on page 23] were edited to remove pendulum-paths in corresponding figures of the book [Som21, Fig. 75 on page 272][Som23, Fig. 72 on page 240].)

Would Bohr's extra rule from 1918 have carried the same weight with Sommerfeld in 1919, if Sommerfeld had assumed that Bohr's rule was an echo of his own earlier opinion from 1915 that he had revised in 1916 or 1917 due to Epstein's work explaining observations of the Stark effect? Probably not. What else would have changed? Sommerfeld might have quoted Bohr's extra rule less often, which was what actually happened in later editions of his book [Som23], but he still argued that pendulum-paths should be excluded due to collisions with the nucleus. In any case, the anecdote might serve as a reminder that even great physicists (like Sommerfeld and Bohr) might fall victim to confirmation bias and echo chambers.

Soon after the Bohr-Sommerfeld model of atoms was published, modern quantum mechanics established the existence of states of hydrogen-like atoms with zero orbital angular momentum [PW35]. Pendulum-paths are not only the natural representation of such states in the Bohr-Sommerfeld model but also in many interpretations of quantum mechanics that include electron trajectories, e.g., ensemble interpretations [Bal70]. Therefore, it is not surprising that several researchers revisited the idea of pendulum-paths in hydrogen-like atoms since the 1920s, for example, Nicholson [Nic23], Lindsay [Lin27], Pauling [PW35, Pau60], Dankel and Levy [DL74], Bucher [Buc06, Buc08], and Rivas [Riv24]. Interested readers may find many more details about the history of pendulum-path (including pendulum-paths in two-electron systems) in Bucher's work [Buc08].

3 Simulation of Spinning Electrons on Pendulum-Paths

According to Rivas [Riv24], a spinning electron on a pendulum-path in a hydrogen atom spirals around the nucleus without colliding with it (see Section 2.1). The numerical simulation of this scenario

theoretisch begründetes Auswahlprinzip zusammen mit dem Bohrschen Verbot der verschwindenden äquatorialen Quantenzahlen. Epstein dagegen benutzte ein (vom Verfasser früher vertretenes, jetzt fallen gelassenes) mehr empirisches Auswahlprinzip." [Som21, pages 451–452]

[5] Original passage in German: „die Kreisbahn, die wir jedenfalls als möglich erklären werden" [Som15b, page 445]

presented here was based on the following equations of motion of Beck's model of a spinning electron [Bec23]:

$$\ddot{x}^\mu = -\omega_0^2 \, (x^\mu - y^\mu) \,, \tag{1}$$

$$\ddot{y}^\mu = \frac{q}{m} F^{\mu\nu}(x) \, \dot{x}_\nu, \tag{2}$$

where the 4-vector $x(\tau) = (c\,t, \mathbf{x})$ describes the space-time position of a point-like charge q (i.e., the center of charge) in an observer's inertial reference frame as a function of proper time τ measured by a clock in a rest frame fixed at the electron's spin center, overhead dots denote derivatives with respect to this proper time τ, the 4-vector $y(\tau) = (c\,t_y, \mathbf{y})$ describes the space-time position of the spin center (or center of mass) of a point-like electron of mass m, the angular frequency $\omega_0 = 2\,m\,c^2/\hbar$ is twice the angular Compton frequency of electrons, c is the speed of light, $\hbar = h/(2\pi)$ is the reduced Planck constant, and $F(x)$ denotes the electromagnetic field tensor at the space-time position of the center of charge x.

Additionally, two constraints have to be satisfied: The first constraint

$$\dot{x}_\mu \dot{x}^\mu = 0 \tag{3}$$

requires electrons to move at the speed of light c. The second constraint

$$\ddot{x}_\mu \ddot{x}^\mu = -c^2 \omega_0^2 \tag{4}$$

requires free electrons to orbit the spin center (in the rest frame of this spin center) at an angular frequency of ω_0 on a circular path with radius $r_0 = c/\omega_0$.

Furthermore, the present work assumes $x^0 - y^0 = c\,t - c\,t_y \approx 0$ for electrons on pendulum-paths in hydrogen atoms. In this approximation, the local spin motion $x(\tau) - y(\tau)$ is limited to a plane orthogonal to the velocity of the spin center. Thus, it is sufficient to integrate $y(\tau)$ as if it described a spinless, relativistic electron accelerated by an electromagnetic force—except that this electromagnetic force is evaluated for $x(\tau)$ instead of $y(\tau)$. $x(\tau)$, on the other hand, may be integrated by advancing the circular spin motion with radius r_0 and time-dilated angular frequency ω_0/γ in the rest frame of the spin center in a plane orthogonal to the velocity of the spin center, where the Lorentz factor γ is determined by the velocity of the spin center in the observer's reference frame.

For the actual numerical integration method, an explicit midpoint method was implemented. The step size was chosen small enough to allow for multiple integration steps per period of the spin motion. After each (full) step of this midpoint method, the sum of the kinetic and potential energy of the electron (as represented by the motion of the spin center) was computed. When this sum differed sufficiently from the initial energy, the velocity of the spin center was adjusted such that the sum of the kinetic and potential energy of the electron remained approximately constant. This energy-based correction usually prevents the solution from diverging or collapsing into the nucleus, but it does not necessarily improve the accuracy of the computed trajectory. Since this correction is numerically instable for very small velocities, it was skipped for very small velocities relative to the speed of light—specifically, near the turning points of pendulum-paths.

The arbitrarily small velocity of the spin center at turning points of pendulum-paths may also cause an issue with the integration of the local spin motion $x(\tau) - y(\tau)$ at those points. If the local spin motion is always limited to a plane orthogonal to the velocity of the spin center, then a spinning electron on a path sufficiently close to a perfectly straight pendulum-path is changing its helicity each time the spin center moves through a turning point. In some sense, the electron spins on the spot of the turning point for a moment, and then the spin center continues its path, but toward the nucleus instead of away from it. In this process, a spinning electron on a pendulum-path naturally changes its helicity at each turning point. The implemented integration of the local spin motion allows for this process by continuously updating a three-dimensional vector variable for the spin axis (with handedness) to be either parallel or anti-parallel with the velocity of the spin center depending on which alignment requires the smaller rotation of the previous value of the spin axis. This vector variable is continuously updated except when the velocity of the spin center is too small to provide a numerically reliable direction, in which case the value of the spin axis is temporarily preserved.

In order to simulate the equations of motion of spinning electrons proposed by Kraus [Kra24], the value of ω_0 has to be changed to $\omega_1 = m\,c^2/\hbar$ and the value of r_0 has to be changed to $r_1 = c/\omega_1$.

4 Results

The first result obtained by the simulation was that a spinning electron on a pendulum-path in a hydrogen atom is in fact spiraling around the nucleus without "falling" into it. The maximum distance of the simulated electron on a pendulum-path as well as the time period from perihelion to perihelion numerically matched the expected values for pendulum-paths [DL74, Buc06]. This provided numerical evidence that spinning electrons can serve as a plausible explanation of how electrons move on pendulum-paths—as already hypothesized by Rivas [Riv24].

Inspired by Pauling and Wilson [PW35], the trajectories of a simulated electron on pendulum-paths (azimuthal quantum number $l = 0$) in a hydrogen atom (atomic number $Z = 1$) for values 1, 2, and 3 of the principal quantum number n were further analyzed by evaluating time-averaged values $\overline{r}$, $\overline{r^2}$, $\overline{r^{-1}}$, and $\overline{r^{-2}}$ of powers of the distance r between the fixed position of the nucleus and the center of charge of the spinning electron. (Using the center of mass instead of the center of charge resulted in worse results, specifically for $\overline{r^{-1}}$ and in particular for $\overline{r^{-2}}$, which is not surprising considering that the center of mass moves straight through the nucleus.)

Pauling and Wilson [PW35, page 144] provided the time-averaged value $\overline{r_{nk}}$ for a Bohr-Sommerfeld orbit with principal quantum number n and azimuthal quantum number k as

$$\overline{r_{nk}} = \frac{n^2 a_0}{Z}\left(1 + \frac{1}{2}\left(1 - \frac{k^2}{n^2}\right)\right) \tag{5}$$

with the Bohr radius a_0. For an improved version of the Bohr-Sommerfeld model, Pauling and Wilson suggested replacing k^2 by $l(l+1)$ with values $l = 0, \ldots, n-1$. The resulting expression is identical to the expectation value of r_{nlm} in a basic hydrogen model in non-relativistic quantum mechanics (i.e., "wave mechanics") [PW35, page 144].

In all simulated scenarios ($Z = 1$; $n = 1, 2, 3$; $l = k = 0$), numerical results for $\overline{r}$ matched the expected values with deviations of less than 1%. Results obtained with the model by Beck [Bec23] were slightly worse than those obtained with the model by Kraus [Kra24] but still within 1% of the expected values.

For the time-averaged value $\overline{r_{nk}^2}$ in the Bohr-Sommerfeld model, Pauling and Wilson [PW35, page 145] provided the expression

$$\overline{r_{nk}^2} = \frac{a_0^2 n^4}{Z^2}\left(1 + \frac{3}{2}\left(1 - \frac{k^2}{n^2}\right)\right) \tag{6}$$

while the non-relativistic quantum-mechanical model predicts [PW35, page 144]

$$\overline{r_{nlm}^2} = \frac{a_0^2 n^4}{Z^2}\left(1 + \frac{3}{2}\left(1 - \frac{l(l+1) - \frac{1}{3}}{n^2}\right)\right). \tag{7}$$

Thus, even for $k = l = 0$, $\overline{r_{nk}^2}$ is less than $\overline{r_{nlm}^2}$ by $a_0^2 n^4 Z^{-2}/(2n^2)$.

Numerical results obtained with the models by Beck and by Kraus matched $\overline{r_{nk}^2}$ of the improved Bohr-Sommerfeld model with deviations of less than 1%; therefore, they both systematically underestimated the value of the wave-mechanical $\overline{r_{nlm}^2}$.

The time-averaged value of $\overline{r_n^{-1}}$ in the Bohr-Sommerfeld model as well as in the wave-mechanical model is $Z/(a_0 n^2)$ [PW35, page 145]. Numerical results matched these values with deviations of less than 1%. Here, the model by Beck provided slightly better results than the model by Kraus.

For $\overline{r^{-2}}$, the wave-mechanical model predicts [PW35, page 145]

$$\overline{r_{nlm}^{-2}} = \frac{Z^2}{a_0^2 n^3 (l + \frac{1}{2})}, \tag{8}$$

while the Bohr-Sommerfeld model predicts

$$\overline{r_{nk}^{-2}} = \frac{Z^2}{a_0^2 n^3 k}. \tag{9}$$

Thus, $\overline{r_{nk}^{-2}}$ is undefined in the case $l = k = 0$ of the improved Bohr-Sommerfeld model considered here. Apparently, $\overline{r_{nk}^{-2}}$ is finite for $k = 1$ in the original Bohr-Sommerfeld model, which, however, does not include pendulum-paths.

In comparison to the wave-mechanical value of $\overline{r_{nlm}^{-2}}$, the numerical results obtained with the model by Kraus were too large by a factor of almost 4 while the results obtained with the model by Beck were too large by a factor of almost 5. These larger deviations in the model by Beck are probably a result of the smaller spin radius (by a factor of 2) in his model compared to the model by Kraus.

While deviations by a factor of 4 (or 5) are large, they are an improvement compared to the undefined predictions of the improved Bohr-Sommerfeld model employed by Pauling and Wilson [PW35]. (Arguably, the original Bohr-Sommerfeld model provides better predictions for $\overline{r^{-2}}$ by excluding the case $k = 0$. However, it provides worse predictions for $\overline{r}$ and $\overline{r^2}$. Furthermore, it features additional shortcomings as discussed by Bucher [Buc08].)

5 Conclusions and Future Work

The main objective of this work was to provide numerical evidence for Rivas' hypothesis [Riv24] that spinning electrons can move on paths of zero orbital angular momentum (i.e., pendulum-paths) with the center of mass of the electron moving straight through the nucleus. The numerical simulations showed not only that electrons on pendulum-paths spiral around the nucleus at a safe distance, but also that time-averaged values of powers of the distance between the nucleus and the center of charge of electrons on pendulum-paths are closer to the corresponding quantum mechanical expectation values than for an improved variant of the Bohr-Sommerfeld model [PW35, Buc06]. Furthermore, the discussion in Section 2.2 of the historical circumstances of the exclusion of pendulum-paths in the original Bohr-Sommerfeld model shows that there might have never been any compelling scientific reason to exclude them in the "old quantum theory." In modern quantum mechanics, on the other hand, the reality of particle trajectories in general is often denied or the concept is declared meaningless for quantum mechanics. However, some interpretations of quantum mechanics (in particular ensemble interpretations) assume the existence of particle trajectories; thus, pendulum-paths might still have an important role to play in quantum mechanics.

Future work includes improvements of the numerical simulation (in particular considering the approximation $t - t_y \approx 0$, which is assumed in this work but might not be justified for all trajectories of electrons in atoms) and further applications of the numerical simulation; for example, other atoms than hydrogen as well as bound states of pairs of electrons [Riv24].

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A Revisions

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