How the modified Bertrand theorem explains regularities of the periodic table I. From conformal invariance to Hopf mapping

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Abstract

Bertrand theorem permits closed orbits in 3d Euclidean space only for 2 types of central potentials. These are of Kepler- Coulomb and harmonic oscillator type. Volker Perlick recently extended Bertrand theorem. He designed new static spherically symmetric (Bertrand) spacetimes obeying Einstein’s equations and supporting closed orbits. In this work we prove that the topology and geometry of these spacetimes permits to solve quantum many-body problem for any atom of periodic system exactly. The computations of spectrum for any atom of periodic system becomes analogous to that for hydrogen atom. Initially the exact solution of the Schrödinger equation for any multielectron atom was obtained by Tietz in 1956. However, neither himself nor others fully comprehended what actually was obtained. We recalculated Tietz results by applying the methodology consistent with new (different from that developed by Fock in 1936) way of solving Schrödinger’s equation for hydrogen atom. In the light of this new result it had become possible to demonstrate rigorously that the Tietz- type Schrödinger’s equation is in fact describing the quantum motion in Bertrand spacetime. As a bonus, we obtained the analytical proof of the Madelung rule thus solving the Löwdin’s challenge problem.

Keywords

Maxwell’s fish-eye potential, conformally invariant classical and quantum equations, superintegrability, quantum Bertrand spacetimes

1. Background and summary

1.1. Overview of trends in description of the periodic system of elements.

Statement of Löwdin’s challenge problem

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Although quantum mechanical description of multielectron atoms and molecules is considered to be a well established domain of research in quantum mechanics, recently published book [1] indicates that there are still many things which are left for development. Even though the cited book represents a significant step towards improvement of the existing description of electron structure of atoms and molecules, we were able to find many other items requiring further study. As is well known, the quantum mechanical description of multielectron atom (with atomic number $Z$ and infinitely heavy nucleus) begins with writing down the stationary Schrödinger equation

$$\hat{H}\Psi(r_1, r_2, \ldots, r_Z) = E\Psi(r_1, r_2, \ldots, r_Z)$$ (1.1a)

with Hamiltonian

$$\hat{H} = -\sum_{i=1}^{Z}\frac{\hbar^2}{2m}\nabla_i^2 - \sum_{i=1}^{Z}\frac{Ze^2}{r_i} + \frac{1}{2}\sum_{i,j=1, i\neq j}^{Z}\frac{e^2}{r_{ij}}.$$ (1.1b)

Following Bohr’s Aufbauprinzip the atom with atomic number $Z$ is made up of electrons added in succession to the bare atomic nucleus. At the initial stages of this process electrons are assumed to occupy the one-electron levels of lowest energy. This process is described in terms of the one electron eigenvalue problem

$$\hat{H}_i\psi_{\Box_i}(r_i) = [-\frac{\hbar^2}{2m}\nabla_i^2 + V_{\text{eff}}(r_i)]\psi_{\Box_i}(r_i) = \varepsilon_{nl}(i)\psi_{\Box_i}(r_i), i = 1 \div Z,$$ (1.2)

where $V_{\text{eff}}(r_i)$ is made of the combined nuclear potential $-\frac{Ze^2}{r_i}$ for the $i$-th electron and the centrally symmetric Hartree-Fock type potential $F(r_i)$ coming from the presence of the rest of atomic electrons. The fact that $F(r_i)$ is indeed centrally symmetric was discussed in the book by Bethe and Jackiw [2]. Later on, in the text and, especially in the Appendix G, we provide much more details on this topic. The symbol $\Box_i$ indicates the $i$-th entry into the set made out of hydrogen-like quantum numbers characterizing individual electrons. Recall that the concept of orbital is determined by the major quantum number $n$ having its origin in studies of hydrogen atom. The number of electrons allowed to sit on a given orbital is determined by the Pauli exclusion principle. Thus, with increasing $Z$ electrons are occupying successive orbitals according to Bohr’s Aufbau scheme until the final ground state electron configuration is reached. Since electrons are indistinguishable, the hydrogen-like quantum numbers $n, l, m$ and $m_s$ cannot be associated with a particular electron. Therefore, the symbol $\Box_i$ should be understood as representing a specific set of quantum numbers otherwise used for description of individual (that is not collectivized) electrons.

The problem with just described Aufbauprinzip lies in the assumption that the guiding principle in designing the final ground state electron configuration is made out of two components: a) knowledge of hydrogen atom-like wave functions supplying the quantum boxes/numbers $\Box_i$ and, b) the Pauli principle which is mathematically restated in the form of the fully antisymmetric wavefunction $\Psi(r_1, r_2, \ldots, r_Z)$. Should these requirements be sufficient, then it probably would be possible with good accuracy to replace $V_{\text{eff}}(r_i)$ by $-\frac{Ze^2}{r_i}$ so that the filling of electronic levels would occur according to the Fock $n$-rule.
Fock n-rule: With increasing $Z$ the $nl$ orbitals are filled in order of increasing $n$.

This rule leads to the problems already for the lithium as explained in [1], page 330. As result, the $(n,l)$ rule was proposed instead.

The hydrogenic $(n,l)$ rule: With increasing $Z$, the orbitals are filled in order of increasing $n$ while for a fixed $n$ the orbitals are filled in order of increasing $l$.

After $Z = 18$ the $(n,l)$ rule breaks down though. Therefore, it was subsequently replaced by the $(n + l, n)$ rule suggested by Madelung- the person who reformulated Schrödinger’s equation in hydrodynamic form [3].

The Madelung $(n+l,n)$ rule: With increasing $Z$, the orbitals are filled in order of increasing $n+l = N$. For fixed $N$, the orbitals are filled in order of increasing $n$.

All the above rules are empirical. As such, they require theoretical explanation. This fact brings us to the

Löwdin’s challenge problem: Find a way to derive the Madelung rule ab initio.\footnote{This problem was posed by Per-Olov Löwdin [4]. Additional details and references are given in [5].}

The essence of Mendeleev’s periodic system of elements lies exactly in discovered periodicity of properties of chemical elements. Although there are 100’s of ways this periodicity is exhibited\footnote{Results of www searches indicate that this process is still ongoing.}, the commonly accepted periodic table of elements consists of seven periods: 2-8-18-18-32-32. Notice that all period lengths occur in pairs (period doubling), except for the very first period of size 2. To determine whether this exception is intrinsic or not, analysis of work by Charles Janet on periodic table done in 1930 (6 years before work by Madelung!) is the most helpful, [1], pages 336-340. Although initially Janet developed his version of periodic table without guidance of quantum mechanics, eventually he did make a connection with Bohr’s results. Janet’s periodic table has 8 periods. The periods in Janet’s table are characterized (without exception) by the constant value of $N = n + l$. It is in excellent agreement with the Madelung rule suggesting elevation of $N = n + l$ to the rank of new quantum number. By organizing the elements in periods of constant $n+l$ and groups of constant $l, m_l$ and $m_s$, the period doubling emerges naturally and leads to the sequence of periods: 2-2-8-18-18-32-32.

1.2. Work by Demkov and Ostrovsky (a gentle introduction)

A concise and convincing explanation of the period doubling and its connection with the Madelung rule is given in [6]. The Madelung rule had attracted the attention of Demkov and Ostrovsky in 1971 resulting in their publication [7] of major importance. Nevertheless, subsequently Kitagawara and Barut [8,9] found apparent flaws in the logic of Demkov-Ostrovsky calculations. The authors of the book [1] also expressed their objections to the Demkov-Ostrovsky cycle of works. On page 381 of [1] we found the following statement: ”Demkov and Ostrovsky developed an atomic physics model that incorporates the Madelung rule, but
by replacing the quantization of level energies with quantization of coupling constants at zero energy.” Furthermore, Demkov and Ostrovsky, while obtained the correct results, had been unable to provide their rigorous justification since their effective potential $V_{eff}(r)$ was correctly guessed. The authors of [1] conclude that, even though the Demkov-Ostrovsky results do reproduce the Madelung rule correctly, the way these results were obtained cannot be considered as solution of the Löwdin challenge. This circumstance brings us to the following

1.3. Summary of the problems to be solved

1.3.1. General background

In this work we demonstrate that the objections raised in [1,8,9] are coming from the lack of knowledge of needed mathematical apparatus by physics and chemistry community, including Demkov and Ostrovsky themselves. In mathematical physics community this apparatus is already known in many other contexts. Thus, one of the tasks of this work is to introduce this apparatus to the atomic and molecular physics community. By doing so a number of problems of major importance is solved and all of the objections raised in [1,8,9] are removed. Some additional objections to be described shortly below are also removed.

In their seminal work [7] Demkov-Ostrovsky (D-O) realized that the key to success of solving problems of periodic table lies is Eq.(1.2) where $V_{eff}(r)$ should be correctly chosen. The Bertrand theorem of classical mechanics [10] imposes seemingly insurmountable restrictions on selection of $V_{eff}(r)$ since for spherically symmetric potentials only the Coulombic $\frac{Ze^2}{r}$ and the harmonic oscillator $kr^2$ potentials allow dynamically closed orbits. D-O believed that, in spite of the indistinguishability of electrons, the discrete spectrum of multielectron atoms should be associated with closed orbits. From the point of view of theory of chaos at the semiclassical level of description the role of closed orbits recently was discussed, e.g. in [11] and, much earlier, in the seminal book by Gutzwiller [12].

1.3.2. Arguments leading to extension of the classical Bertrand theorem

Hoping to bypass limitations of the Bertrand theorem, D-O employed the optical-mechanical analogy in their calculations. It permitted them to use the Maxwell fish-eye potential (and, later on, its conformally deformed modifications) instead of the Coulombic potential. They demonstrated in [7] the equivalence at the classical level between the Hamilton-Jacobi equations employing these two, seemingly different, potentials. D-O hoped that use of the fish-eye potential (or its conformal modification) might allow to bypass limitations of the Bertrand theorem. This fact attracted attention of John Wheeler who in [14,16] and, with his student,

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5 Made of Parts I and II.
6 Begining from the motion of electrons in helium, all atomic multielectron systems are believed to be chaotic.
7 See also the book by Cvitanovic [13].
in [15], studied classically and semiclassically the motion in the fish-eye and conformally
deformed fish-eye potentials used by D-O in [7]. The dynamics of electrons in such con-
formally deformed potentials happens to involve orbits which are closed, planar and have
self-intersections. In his paper [17] Ostrovski argued that the self-intersections of orbits do
not contradict the Bertrand theorem. This statement by Ostrovski happens to be wrong
as demonstrated in section 5. In it, we mention works by other authors who obtained the
same results prior to the discovery of curved Bertrand spacetimes. None of these authors
was concerned with the limitations of Bertrand theorem. Very recently, in 2017, the same
self-intersecting patterns were obtained for dynamical trajectories in Bertrand spacetimes,
e.g. see page 3362 of [18]. The results were obtained without any reference to atomic physics.

According to work by Little [19] there are only 3 distinct regular homotopy classes of
oriented closed curves on $S^2$. These are: a) those for curves without self-intersections, b) those
for curves with just 1 self–intersection and, c) those with 2 self-intersections. The b)-type
homotopy class curves were obtained by Wheeler and by other authors as discussed in section
5. Thus, from the work by Little it follows that the effects of curvature and presence of self-
intersection in dynamical trajectories are connected with each other. The Kepler-Coulomb
dynamics in flat 3d Euclidean space does not allow self-intersections. The self-intersections
are allowed if the Bertrand theorem is extended to motions on curved (Bertrand) manifolds
[18]. The sphere $S^2$ is conformally flat. The results of the modified Bertrand theorem are valid
exactly for the conformally flat manifolds. Details are given in section 5. These are corollaries
of results obtained in [20]. Thus, flatness of self-intersecting patterns obtained in [18] is in
fact conformal flatness.

To connect Bertrand spacetimes with atomic physics we begin with D-O statement made
in [7]: "The Maxwell’s fish-eye problem is closely related to the Coulomb problem". Being
aware of the book by Luneburg [21] D-O nevertheless underestimated the nature of
connection between the Coulombic and optical (fish-eye) problems described in [21]. This
fact is discussed in detail in section 2. The assumption of only "close relationship" caused
D-O to replace Eq.(1.2) by

$$\left[-\frac{\hbar^2}{2m}\nabla_i^2 + V_{eff}(r_i)\right]\psi(r_i) = 0.$$  \hspace{1cm} (1.3)

Eq.(1.3) is looking differently from Eq.(1.2). Eq.(1.2) is the eigenvalue problem while Eq.(1.3)
is the Sturmian problem. For such type of problem to make sense the parameters entering
into $V_{eff}(r_i)$ must be quantized. Such quantization of parameters is making Sturmian and
eigenvalue problems equivalent. This fact is nontrivial. It is considered in detail in sections 2
and 4 of Part I and Appendices A,B, E and F. Without further explanations this equivalence
represents the major reason for using the fish-eye-type potentials in treatments of atomic
systems. In fact, in many ways (discussed in section 3 and Appendices C, D and F) to use
Eq.(1.3) is more advantageous than Eq.(1.2).

In [1], page 377, we read that Eq.(1.3) ”does not describe the bound states of the atom”.

\textsuperscript{7}This concept was defined in our work [3] and is going to be also explained in the bulk of this work.

\textsuperscript{8}Ref.4 in [7].
That this is not the case could be concluded already by D-O themselves should they read the corresponding places in books by Lunenburg [21] and Caratheodory [22]. They do quote these works though in [7]. This misunderstanding of importance of Eq.(1.3) and its relation with Eq.(1.2) resulted in critique and neglect of D-O works, e.g. read [1], page 377. In this (two parts) paper we are going to demonstrate that Maxwell’s fish-eye and related to the fish-eye classical and quantum problems are not closely related to the Coulombic (hydrogen atom) problems. Instead, the Maxwell fish-eye problem is isomorphic to the Coulombic problem both classically and quantum mechanically. This is illustrated in section 4. By overlooking the Coulombic-fish-eye isomorphpism at the quantum level D-O argued, nevertheless, that Schrödinger’s Eq.(1.3) with Coulombic and fish-eye-type potentials both possess the O(4,2) dynamical symmetry known for the hydrogen atom and later established for the rest of atoms of the periodic table [1], [3]. Selection of the fish-eye-like potentials by D-O was guided in part by their desire to describe the atoms other than hydrogen. In addition, they believed that: a) $V_{\text{eff}}(r_i)$ in Eq.(1.3) can be represented by the conformally deformed fish-eye potential so that b) use of such potential removes restrictions posed by the Bertrand theorem in flat space. Ostrovsky concludes his paper [17] with the following remark: "It leaves a very interesting question unresolved, the question of why the interaction of a number of electrons with each other and with an atomic nucleus leads to an effective one-electron potential having some approximate hidden symmetry. The method of solution of this question can hardly be envisaged at the present time."

Thus, with complete formal success of quantum description of atoms of the whole periodic system [7] culminating in formal proof of the Madelung rule, Ostrovsky admits that with all his results published to date the Löwdin’s challenge problem still remains out of reach. This is so because the deformed fish-eye potential used in D-O calculations had no visible connection with $V_{\text{eff}}(r_i)$ coming from the Hartree-Fock calculations. In addition to their inability of solving the Löwdin challenge, D-O also failed to solve the Bertrand challenge: What makes the deformed fish-eye potential used by D-O as substitute of $V_{\text{eff}}(r_i)$ so good that it removes the restrictions of the classical Bertrand theorem?

1.3.3. Analytical equivalence of the Hartree-Fock $V_{\text{eff}}(r_i)$ and the deformed fish-eye potential. The place of Bertrand spacetimes in this equivalence

In their cycle of works on proving the Madelung rule D-O used the fish-eye ($\gamma = 1$) and conformally deformed ($\gamma \neq 1$) fish-eye potentials

$$V(x, y, z) = - \left( \frac{a}{r} \right)^2 \left[ \frac{n_0}{(r/a)^{\gamma}} + \frac{(r/a)^{\gamma}}{(r/a)^{\gamma}} \right]^2,$$

$$r^2 = x^2 + y^2 + z^2, a = \text{const}, \gamma \text{ is a rational number, as an alternative to the } V_{\text{eff}}(r_i) \text{ Hartree-Fock type potentials routinely used in atomic physics literature. Such a replacement required them to switch from Eq.(1.2) to Eq.(1.3) for reasons explained in detail below, in sections 2 and 3 and Appendices A and B. Since Eq.(1.3) seemingly allows only to look for}$$

\[\text{...that is the group-theoretical (our insert from previous discussion) consideration...}\]
eigenfunctions with zero eigenvalue, both D-O and the rest of researchers in the field considered this limitation as a serious deficiency. In this work we demonstrate that this restriction is harmless and, in fact very helpful. We remind our readers, that use of the potential, Eq.(1.4), was made by D-O for the purpose of taking care of limitations of the classical Bertrand theorem. No other authors were concerned with these limitations. Apparently, this fact allowed D-O to neglect works by other authors on the same or related subjects and to draw attention of others [1] only to their own works. This happens to be a fundamental drawback. Details are given in section 5 and Appendices F and G.

Below, we provide a brief summary of results just mentioned. D-O realized that when used in Eq.(1.3) the constant \( n_0 \) acquires discrete values as it happens in all Sturmian type problems (Appendix F). Furthermore, for \( \gamma = 1/2 \) the solution of Eq.(1.3) provides results compatible with the Madelung rule. The apparent limitation, \( E = 0 \), along with no apparent relationship between the potential \( V(x, y, z) \) and \( V_{eff}(r) \) coming from the Hartree-Fock calculations caused Ostrovski to acknowledge (in [17]) that all D-O results to date do not solve the Löwdin challenge problem. Thus, we are left with the following (unproven) facts:

a) use of the potential, Eq.(1.4), removes the limitations of classical Bertrand theorem;

b) the choice \( \gamma = 1/2 \) in Eq.(1.4) apparently explains the Madelung rule;

c) finding of the spectral results beyond \( E = 0 \) requires uses of sophisticated perturbational methods;

d) the choice \( \gamma = 1/2 \) in Eq.(1.4) is detached from the Hartree-Fock results;

e) the case \( \gamma = 1 \) corresponds to the standard Maxwell’s fish-eye potential. Classical dynamics in such potential is isomorphic to that in Kepler-Coulomb potential. However, because of the apparent \( E = 0 \) limitation, neither D-O nor other researchers reproduced known eigenvalue spectrum for the hydrogen atom.

Subsequently, other authors studied Eq.(1.3) with D-O potential, Eq.(1.4), in 2 dimensions where use of conformal transformations leaves Eq.(1.3) form-invariant. This fact provides many advantages. Still, no attempts to reproduce known 2 dimensional results for hydrogen atoms were made. In our work we use the observation, in section 4, that results on \( \mathbb{R}^2 \) can be lifted to \( S^2 \) and then lifted further to \( S^3 \) via Hopf mapping. These lifting procedures will be discussed in detail in Part II. Using stereographic projection: from \( S^3 \) to \( \mathbb{R}^3 \), it is possible then to reobtain D-O results done on \( \mathbb{R}^3 \). Even though the connection between the Hartree-Fock and the D-O potential, Eq.(1.4), will be discussed in detail from geometrical and topological perspective in Part II, available results allow us to discuss rigorously such a connection in Part I already. Details are given in Appendix G and section 5. The noticed connection is inseparably linked with the validity of the Madelung rule as also explained in Appendix G and section 5.

Going back to a) we direct our readers attention to work [23] by Volker Perlick. In it the results of classical Bertrand theorem [10] valid in Euclidean 3 space had been generalized to static spherically symmetric spacetimes of general relativity. By design, the motion in such spacetimes takes place on closed orbits. In section 5 we demonstrate that the potential,
Eq. (1.4), indeed removes limitations of the classical Bertrand theorem. However, it is used not in flat Euclidean $\mathbb{R}^3$ but in curved Bertrand spacetimes.

The choice $\gamma = 1/2$ listed in b) and d) is indeed connected directly with results of Hartree-Fock calculations and with Madelung rule. In atomic physics literature the potential, Eq. (1.4), $\gamma = 1/2$, is known as the Tietz potential\(^{10}\). Its origin and many properties are discussed in the book by Flugge [24]. Its remarkable numerical coincidence with the corresponding Hartree-Fock potentials were discussed in many places, e.g. read [25], p. 664, fig. 10. Tietz, the author who invented the Tietz potential, was initially driven by the desire to simplify the Thomas-Fermi (T-F) calculations. Much more analytically cumbersome T-F type potentials were used by Latter [26] in his numerical study of Schrödinger equation spectra of low lying excitations for all atoms of periodic system. Numerical results of Latter had been subsequently analyzed by March. On page 76 of [27] without explicit mention of the Madelung rule he described results by Latter in terms of Madelung rule. After discovery of his potential Tietz used it in the stationary Schrödinger equation, Eq. (1.2), in which $V_{\text{eff}}(\mathbf{r}_i)$ was replaced by the Tietz potential, that is by Eq. (1.4) with $\gamma = 1/2$ [28]. Tietz used Eq. (1.2) in which $E \neq 0$ instead of D-O version of this equation, Eq. (1.3). In the light of results of Appendix F this is permissible. Tietz also recognized that Eq. (1.2) with his potential can be solved exactly. His first attempt to do so was initially made in 1956 [28]. The rest of his attempts is summarized in [29]. The exact solution methods in these works differ in style from that used by D-O. Besides, Tietz used these exact solutions only to check them against the Hartree-Fock results for Mercury ($Z = 80$). In doing so he got a good agreement with the Hartree-Fock results. In this work we prove that the Tietz potential used in [28], [29] is describing the classical and quantum motion in Bertrand spacetimes. Unlike Tietz and, in accord with D-O, we used Eq. (1.3) for solving the corresponding eigenvalue problem. Our method of solving this equation differs somewhat from that used by D-O though since their method is unable to reproduce the hydrogen atom spectrum (problem e)). Our way of solving Eq. (1.3) with $\gamma = 1/2$ is consistent with our new way (different from that obtained by Fock in 1936 (discussed in [3])) of obtaining the spectrum of hydrogen atom. We were able to reproduce this spectrum correctly also in 2 dimensions. These facts allowed us to bypass entirely the item c) present in D-O works. They also allow us to obtain the low lying spectrum of any atom of periodic system consistent with the Madelung rule.

2. Known and unknown properties of Maxwell’s fish-eye lenses and potentials associated with them. Their role in optics and quantum mechanics

2.1. Basic facts

Maxwell’s fish eye lens was invented by James Clerk Maxwell. It is nicely described in [6],[30-32]. Its invention was motivated by the desire to make perfect (absolute) optical instrument. In such an instrument it is expected that all rays leaving point $\mathbf{x}$ meet again

\(^{10}\)It is bearing the name of its creator.
at the (conjugated or focal) point $\mathbf{x}'$. Mathematically this can be expressed with help of the Fermat principle. It is described as follows.

Introduce the optical path length $S(\mathbf{x}, \mathbf{x}')$ via the length functional

$$S(\mathbf{x}, \mathbf{x}') = \int_0^t dl,$$

(2.1)

where the conformally flat metric $dl^2$ is given by $dl^2 = n^2(\mathbf{x}(t)) \left( \frac{dx}{dt} \right)^2 dt^2$ with $n(\mathbf{x}(t))$ being position-dependent refractive index of the medium.

**Fermat principle:** Light rays through spatial points $\mathbf{x}(0)$ and $\mathbf{x}'(t)$ move on optically shortest paths.

Based on this definition, it follows that minimization of the functional, Eq.(2.1), results in the Euler-Lagrange equations for geodesics in the optical medium in analogy with equations for the point-like particle moving in the gravitational field [33]. We shall demonstrate below that such noticed known optical-mechanical-gravitational correspondence is capable of producing new results.

Being armed with the above information, now we are in the position to describe the origins of Maxwell’s fish-eye lens. Additional information is given in Appendix A where we discuss relevant work of Constantin Caratheodory. For this purpose, let us consider the $n-$dimensional sphere $S^n$ in the flat Euclidean space $\mathbb{R}^{n+1}$. It is described by

$$S^n = \{(z_1, ..., z_n; y) \mid \sum_{i=1}^n z_i^2 + y^2 = 1\}.$$

(2.2)

The stereographic projection: from $\mathbb{R}^n$ to $S^n$, is given by

$$z_i = \frac{x_i}{1 + \frac{1}{4}x^2}, y = \frac{1 - \frac{1}{4}x^2}{1 + \frac{1}{4}x^2}, i = 1 \div n, x_i \in \mathbb{R}^n, x^2 = x_i x^i.$$

(2.3)

Here and below the summation over repeated indices is assumed. From the mathematical literature [34] it is known that the stereographic projection is a conformal mapping since it is angle-preserving. This means that using Eq.(2.3) it is possible to rewrite the metric $ds^2$ on the sphere $S^n$ in terms of the metric on $\mathbb{R}^n$, that is

$$ds^2_{S^n} = \rho(\{x_i\}) (dx)^2,$$

(2.4a)

where

$$\rho(\{x_i\}) = \left( \frac{1}{1 + \frac{1}{4}x^2} \right)^2.$$

(2.4b)
An example of such relation, e.g. between the metric of the 2-sphere $S^2$ and the metric of the 2-plane $\mathbb{R}^2$ is described in detail in [35], page 88. Since $\mathbb{R}^2 + \{\infty\} = S^2$. The same is true for the spheres of any dimension. The geodesics on $S^n$ are the great circles. All great circles passing through some point $P$ on $S^n$ intersect again in the conjugate point $P'$, that is in the diametrally opposite point $-P$ (the antipodal map [34]). This circumstance can be used for design of perfect optical instruments. Specifically, let us adopt Eq.(2.4a) to 4 and 3 dimensions respectively. Then, in view of Eq.(2.1), the conformal factor $\rho(\{x_i\})$ can be interpreted as the square of refractive index $n^2(x(t))$. This explains the origin of Maxwell’s fish-eye refractive index. Written with account of dimensionality arguments, the refractive index is given by

$$n(x) = \frac{n_0}{1 + x^2/a^2}. \quad (2.5)$$

The light rays in 3 dimensional Maxwell’s fish-eye medium are images of the great circles that is of the geodesics in $S^3$. The antipodal map $P \rightarrow -P, P \in S^3$, corresponds to the negative inversion map $x_i = -\frac{x_i}{|x|^2}, x_i \in \mathbb{R}^3$ from $\mathbb{R}^3$ to $\mathbb{R}^3[52]$. The antipodal points on $S^3$ correspond to points $x_1$ and $x_2$ in $\mathbb{R}^3$ which lie on a common line through the origin, and satisfy $x_1 \cdot x_2 = -1$. The great circles on $S^3$ (that is the geodesics) are just those circles (or lines through the origin in $\mathbb{R}^3$) which map into themselves under the negative inversion operation [34].

These facts, we hope, remind our readers about the classical (by Moser [37, 38]) and quantum mechanical (Fock [39]) treatments of hydrogen atom respectively. They were discussed to a some extent in our previous work [3]. The connection between the description of optical (fish-eye refractive index) instruments and the classical/quantum mechanical description of hydrogen atom was discovered by Luneburg [31]. Some important additional details (not of quantum mechanical nature though) were independently developed by Caratheodory [32]. They are discussed in Appendix A.

Contrary to the D-O claim that the Maxwell’s fish-eye and the Coulomb (that is hydrogen atom) problems are "closely related" [31], Luneburg found the exact mapping between these problems. To avoid further literature interpretation ambiguities, we present Luneburg’s arguments below.

2.2. Luneburg map. Essentials

To shorten our exposition to absolute minimum, we shall use extensively the results of our previous work [3]. It also uses results of Luneburg’s book [31], albeit with different purpose. Thus, we begin with Eq.(4.11) of [3] for the wavefront. We write it in Luneburg’s notations (e.g. see Eq.(28.13) of [31]),

$$\psi_x^2 + \psi_y^2 + \psi_z^2 = n^2(x, y, z) \quad (2.6)$$

and select for the refractive index

$$n^2(x, y, z) = C + \frac{1}{\sqrt{x^2 + y^2 + z^2}}. \quad (2.7)$$
If this equation is to be used in quantum mechanics, Eq. (2.6) must be rewritten in the form of Eq. (4.21) of [31], that is in the form
\[ \psi_x^2 + \psi_y^2 + \psi_z^2 = 2m(E - V) \] (2.8a)

Then, following Schrödinger, the fully reversible substitution: \( \psi \leftrightarrow \hbar \ln \varphi \) done in Eq. (2.8a) is converting it into Eq. (4.22) of [3]. That is into
\[ \varphi_x^2 + \varphi_y^2 + \varphi_z^2 = \frac{2m}{\hbar^2} (E - V) \varphi^2. \] (2.8b)

Eqs. (2.8a) and (2.8b) are equivalent classical Hamilton Jacobi (H-J) equations even though Eq. (2.8b) has \( \hbar \) in it! The rationale of rewriting Eq. (2.8a) into Eq. (2.8b) lies in the fact that the stationary Schrödinger equation is obtainable from Eq. (2.8b) variationally. That is by minimization of the functional
\[ J[\varphi] = \frac{1}{2} \int d^3x [(\nabla \varphi)^2 - \frac{2m}{\hbar^2} (E - V) \varphi^2] \] (2.9)

under subsidiary condition
\[ \int d^3x \varphi^2 = 1 \] (2.10)

the Schrödinger equation
\[ \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \varphi + \frac{2m}{\hbar^2} (E - V) \varphi = 0 \] (2.11)
is obtained. As discussed in [3] the quantum solutions of Eq. (2.11) are also exact solutions of the classical Eqs. (2.8a), (2.8b). Because of this, it is sufficient to look for solutions of quantum Schrodinger’s equation by using classical H-J Eqs. (2.8). This fundamentally nontrivial fact was exploited by Luneburg and was apparently overlooked by Dementov and Ostrovsky who wrote [7] that "Maxwell’s fish-eye problem is closely related to the Coulomb problem".

By comparing Eqs. (2.6), (2.7) with Eq. (2.8a) we realize that Luneburg selected the system of units in which \( C = E, 2m = 1 \) and \( e^2 = 1 \). We hope that his choice should not cause any difficulty in reading. Therefore, we shall proceed along with Luneburg’s choices for the time being. Furthermore, Luneburg in addition performs the following nontrivial Legendre transformation (which is canonical in nature as it will be explained below)
\[ \xi = \psi_x, \eta = \psi_y, \zeta = \psi_z, \]
\[ x = \omega_x, y = \omega_y, z = \omega_z, \]
\[ \psi + \omega = x\xi + y\eta + z\zeta \] (2.12)
resulting in
\[ \xi^2 + \eta^2 + \zeta^2 = C + \frac{1}{\sqrt{\omega_x^2 + \omega_y^2 + \omega_z^2}} \] (2.13a)
or, equivalently,
\[
\omega_\xi^2 + \omega_y^2 + \omega_z^2 = \left( \frac{1}{-C + \xi^2 + \eta^2 + \zeta^2} \right)^2. \tag{2.13b}
\]

By comparing Eqs (2.5)-(2.7) and (2.13) we realize that for negative energies, \( C = -|E| \).
That is presence of the constant \( C \) accounts for the spectrum of bound states of the Coulomb (hydrogen atom) problem. The r.h.s. of Eq (2.13) is describing the fish-eye potential. Luneburg choice \( C = -1 \) apparently caused Demkov and Ostrovsky to conclude that the Schrödinger equation originating from the quantum version of the H-J Eq (2.13b) employing the fish-eye potential should be written with \( E = 0 \) (not to be confused with the choices for \( C \), though). This conclusion is correct and is of fundamental importance to all discussions which follow. However, it is still fundamentally misleading since the condition \( E = 0 \) for the Schrödinger equation with the fish-eye potential is not related to the energy of the Coulombic problem as we just demonstrated! Much more is presented in section 4 and Appendix F. Alternative arguments are presented below.

Specifically, we write the Schrödinger equation with the fish-eye potential as
\[
\left( -\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - \left( \frac{n_0}{|E| + x^2 + y^2 + z^2} \right)^2 \right) \psi = 0 \tag{2.14a}
\]
or, accounting for the discreteness of \(|E| \equiv A\), as
\[
\left( -\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \frac{1}{A} - \left( \frac{n_0}{A} \right)^2 \left( \frac{1}{1 + x^2/A + y^2/A + z^2/A} \right)^2 \right) \psi = 0,
\]
or, equivalently,
\[
\left( -\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - \beta_n \left( \frac{1}{1 + x^2/A + y^2/A + z^2/A} \right)^2 \right) \psi = 0 \tag{2.14b}
\]
resulting in the manifestly discrete constant \( \beta_n \approx \frac{n_0^2}{A^2} \). To make a comparison with the Schrödinger equation for hydrogen atom, in view of Eqs (2.11),(2.13), we have: a) to choose system of units in which \( \hbar = 1 \), b) to replace \( n_0 \) by \( Ze^2 \), c) to multiply the Laplacian by factor of 1/2 (kinetic energy standard form). The combination \( \beta_n \approx \frac{n_0^2}{A^2} \) is then being replaced by\( \beta_n = \frac{(Ze)^2}{|E_n|} \).

In the case of 2 dimensions the discrete values of \( \beta_n \) were calculated by Makowski and Gorska [39]. The reason why this was done in two dimensions is worthy of discussion. We shall do so in sections 3 and 4 and Appendix F.

\footnote{The problem of solving the Schrödinger equation resulting in discretness of \( \beta_n \) is known as Sturmian problem. It is further discussed in section 4 and Appendix F.}
2.3. Lenz and Luneburg generalization of the fish-eye potential

The extension of idea of designing perfect optical instrument is based on the assumption that typically such instruments are axially symmetric. Also, the Euclidean space $\mathbb{R}^3$ in which the fish-eye potential lives can be foliated by the two-spheres $S^2$. The stereographic projection Eqs.(2.2),(2.3) adopted to $S^2$ in notations of Luneburg [31] reads

$$X = \frac{2x}{1 + r^2}, Y = \frac{2y}{1 + r^2}, Z = \frac{1 - r^2}{1 + r^2}, r^2 = x^2 + y^2, \quad (2.15)$$

so that the metric is converted into

$$ds^2 = dX^2 + dY^2 + dZ^2 = 4 \left( \frac{dx}{1 + r^2} \right)^2 + 4 \left( \frac{dy}{1 + r^2} \right)^2 + \left( \frac{d\sqrt{1 - r^2}}{r^2 + 1} \right)^2 = \frac{4}{(1 + r^2)^2} (dx^2 + dy^2). \quad (2.16)$$

In view of axial symmetry it is possible to replace Eqs.(2.4a),(2.4b) by their 2-dimensional analog

$$ds^2 = n^2(x, y)(dx^2 + dy^2), n^2(x, y) = \frac{4}{(1 + r^2)^2}. \quad (2.17)$$

Let now

$$x = u(\xi, \eta), y = v(\xi, \eta). \quad (2.18)$$

and introduce a complex $z$-plane variable via

$$z = f(\xi + i\eta) = u(\xi, \eta) + iv(\xi, \eta). \quad (2.19)$$

The Cauchy-Riemann equations imply

$$|dz|^2 = (dx^2 + dy^2) = |f_z(z)|^2 \left( d\xi^2 + d\eta^2 \right) \text{ with } |f_z(z)|^2 = u_\xi^2 + v_\xi^2 = u_\eta^2 + v_\eta^2 \quad (2.20)$$

By comparing Eqs.(2.17),(2.20) we obtain:

$$n(\xi, \eta) = \frac{2}{1 + r^2} |f_z(z)| = \frac{2}{1 + |f(z)|^2} |f_z(z)|. \quad (2.21)$$

Consider now $f(z) = z^\gamma$, $\gamma \geq 1$. Using Eq.(2.21), we obtain,

$$n(r) = \frac{2\gamma r^{\gamma - 1}}{1 + r^{2\gamma}}. \quad (2.22)$$

For $\gamma = 1$ we recover the fish-eye potential reduced to 2-dimensional space defined in Eq.(2.17). Since $r = \sqrt{x^2 + y^2}$, it is apparently permissible\footnote{Actually, it is not permissible!. The rest of our 2 parts work is devoted to correction of this unintentional error by D-O.} by continuity and complementarity to extend this result to 3 dimensions as it was done by D-O and the rest of authors.
who followed D-O to obtain the extended fish-eye like potential (index of refraction) in 3 dimensions
\[ n(r) = \frac{\beta_n (r/a)^{\gamma^{-1}}}{1 + (r/a)^{2\gamma}} = \frac{a}{r^{\gamma} (r/a)^{\gamma} + (r/a)^{\gamma}}. \]  
(2.23)

Here \( r = \sqrt{x^2 + y^2 + z^2} \). The constant \( a \) making the ratio dimensionless is specified in section 4. The \( n(r) \) defined by Eq.(2.23) should not be confused with the analogous result used in 2 dimensional calculations. For \( \gamma = 1 \), by design, such a potential coincides with that presented in Eq.(2.5) as required. The D-O potential, used for the whole periodic system, is obtained by selecting \( \gamma = 1/2 \) in Eq.(2.23). This choice is motivated by some classical and semiclassical arguments apparently allowing to by-pass restrictions of the classical Bertrand theorem. This hypothesis by D-O is incorrect in the form discussed by D-O. Instead, it is studied in detail in section 5 from the point of view of Bertrand spaces. There are yet other, less sophisticated, arguments causing selection of the exponent \( \gamma = 1/2 \). First of them lies in the fact that only for such exponent it is possible to repeat word-for-word scaling calculations done in Eq.s(2.14 a) and (2.14b) and to get the quantization of the coupling constant \( \beta_n \) in a manner used for the fish-eye potential. Such a quantization was postulated by D-O. They entirely overlooked the scaling analysis. Second of them lies in the observation that, when used in the Schrödinger Eq.(2.14), such a potential coincides exactly (up to scaling) with that proposed by Tietz [24] as discussed in section 1 and Tietz potential wonderfully coincides with that obtained with help of the Hartee-Fock calculations [25].

2.4. Contributions of Constantin Caratheodory into design of perfect optical instruments evaluated from the modern theoretical perspective

2.4.1. Connections with the work by Dirac on the theory of constraints and the problem of time in quantum mechanics, quantum field theory and gravity

Eq.(A.5) of Appendix A coincides exactly with Eq.(3.4) of lecture notes by Dirac [41] on quantum mechanics and theory of constraints. It is also given in Part II, section 4, of the classical book by Arnol’d [42]. More is presented in the book by Oliver Johns[43] and in [44]. We follow Ref.s[44] and [45] in which modern treatment of constrained systems is given in the context of gauge fields and time-dependent processes. Thus, in Eq.(A.5) we shall assume that \( t = q_0(\tau) \) so that \( \frac{dt}{d\tau} = \dot{q}_0 \). Using these changes of notations, we obtain as well: \( \dot{q}_i = \frac{dq_i}{d\tau} = \dot{q}_i \frac{dt}{d\tau}, i = 1 \div n \), so that \( L'(t', q'_i, \frac{dq'_i}{dt}) = L^*(\tau, q_i, \dot{q}_i) \). If initially \( L(t, q_i, \dot{q}_i) = \frac{1}{2} g_{ij} \dot{q}_i \dot{q}_j - V(\{q_i\}) \) then, finally we obtain: \( L^*(q_0, q_i, \dot{q}_0, \dot{q}_i) = (\frac{1}{2} g_{ij} \dot{q}_i \dot{q}_j / (\dot{q}_0)^2 - V(\{q_i\}))\dot{q}_0 \).

The canonical momenta now are given as follows:
\[ p_i = \frac{\partial L^*}{\partial \dot{q}_i} = g_{ij} \frac{\dot{q}_i}{\dot{q}_0} \quad \text{and} \quad p_0 = \frac{\partial L^*}{\partial \dot{q}_0} = -\frac{1}{2} g_{ij} \dot{q}_i \dot{q}_j / (\dot{q}_0)^2 - V. \]  
(2.24)

\(^{13}\)See also a paper by Belokolos [40] who used the WKB method applied to Schrodinger’s equation with Tietz potential for proving the validity of the Madelung rule.
Since the first of these equations yields
\[
\frac{\dot{q}_j}{q_0} = g^{ji} p_i,
\] (2.25)
its use in the second of Eqs.(2.24) produces
\[
p_0 + \frac{1}{2} g^{ij} p_i p_j + V = 0 \text{ or } p_0 + H(q_i, p_i) = 0.
\] (2.26)
According to known rules of mechanics, the "true" Hamiltonian \( H(q_\alpha, p_\beta) \), \( \alpha, \beta \in 0 \div n \), is obtainable now via prescription
\[
H(q_\alpha, p_\beta) = p_\alpha \dot{q}_\alpha + p_0 \dot{q}_0 - L^*(q_0, q_i, \dot{q}_0, \dot{q}_i) = \dot{q}_0 (p_0 + \frac{1}{2} g^{ij} p_i p_j + V) = 0.
\] (2.27)
Evidently, the quantized version of just obtained result can formally be written as
\[
H(\hat{q}_\alpha, \hat{p}_\beta) \psi(\{\hat{q}_\alpha\}) = 0,
\] (2.28)
where the hats denote the Hilbert space operators. Eq.(2.14a) belongs to the class of "timeless" equations of the type defined by Eq.(2.28). This circumstance provides us with the opportunity to illustrate general results described by Eqs. (2.27),(2.28) in sufficient detail. These are to be used in the rest of this paper.

2.4.2. Kepler's problem as model example of solution of the time problem

in quantum mechanics

Our readers should be warned that the description of this topic in full generality requires many volumes. For the latest example, e.g. read [46]. In gravitation the story also begins with Eq.(2.26), e.g. read [47], Eq. (1.11). A condensed summary is given in [48] by the same author. To keep focus on tasks to be completed in this paper, we squeeze general description of time problem to the absolute minimum. We shall study time-related issues using Eq.(2.14b) first because at least in 2 dimensions (rigorously) the fish-eye potential, Eq.(2.5), can be replaced by the Lenz potential, Eq.(2.23), without D-O restrictions to the case of \( \gamma = 1/2 \). This can be achieved because the two dimensional Laplacian is conformally invariant. The conformal transformations leading to extension of the fish-eye potential discussed in subsection 2.3. are fully compatible with those for the two-dimensional Laplacian. This fact allowed both classical and quantum mechanical problems to be studied in detail in [39] and [49]. In 3 dimensions situation seems intractable because the Laplacian is no longer conformally invariant. Therefore, by completely ignoring the issue of conformal invariance the fish-eye potential in Eq.(2.14a) was formally replaced by its 3-dimensional Lenz extension by Ostrovsky [17] and by Barut and Kitagawara [8,9] for the special case \( \gamma = 1/2 \). For arbitrary \( \gamma \geq 1 \) it was studied already in [7] and, later on, in [50], again by totally neglecting the issue of conformal invariance. Thus, in this work we are confronted with the task of relating conformally the Schrödinger Eq.(2.14a), where the fish-eye potential is used legitimately,
with the analogous 3-dimensional Schrodinger’s equation with the Lenz fish-eye-like potential whose use in 3-dimensions is lacking justification thus far.

Our study begins with rewriting Eqs. (2.13), (2.14) classically first. We obtain,

\[ (A + |r|^2)^2 |p|^2 = n_0^2. \]  

(2.29)

Here \( |r|^2 = x^2 + y^2 + z^2 \) and \( |p|^2 = \omega_x^2 + \omega_y^2 + \omega_z^2 \). Up to rescaling \((A + |r|^2)^2 |p|^2\) can be identified with the classical Hamiltonian for the Kepler problem discussed in [51], Eq.(7).

Upon quantization Eq.(2.29) becomes a Sturmian problem. Our task, however, is to bring this result into the form coinciding with Eq.(2.27) and to study the consequences.

For this purpose following [51] we have to perform the canonical transformations analogous to those displayed in (2.12). This time, following [51] and [52], we would like to arrive at our final result more systematically. Thus, we begin with Kepler’s Hamiltonian

\[ H = \frac{1}{2} |p|^2 - \frac{\alpha}{|r|}, \]  

(2.30)

and, using Eqs. (2.26), (2.27), we write

\[ 0 = (H - E) \frac{|r|}{\alpha} = \left( |p|^2 - 2E \right) \frac{|r|}{2\alpha} - 1 \equiv H_0. \]  

(2.31)

In the above equation, following Moser [36], [37], we used the Levi-Civita time change

\[ \frac{dt}{d\tau} = \dot{q}_0 = \frac{|r|}{\alpha} \]  

(2.32)

whose physical meaning is discussed in detail in Appendix B. Again, following Moser [36], [37], and [52], we introduce the new Hamiltonian function \( \mathcal{F} \) via

\[ \mathcal{F} = \frac{1}{2} (1 + H_0)^2 = \frac{1}{8\alpha^2} (|p|^2 - 2E)^2 |r|^2. \]  

(2.33)

But \( H_0 = 0 \)! Therefore, on isoenergetic surface \( H = E \) or, which is the same, on \( \mathcal{F} = \frac{1}{2} \), the trajectories of the Hamiltonian flow of \( H \) traversed in time \( t \) coincide with trajectories of the Hamiltonian flow of \( \mathcal{F} \) traversed in time \( \tau \). Details are provided in Appendix B.

In this subsection, however, we still need to demonstrate that the Hamiltonian \((A + |r|^2)^2 |p|^2\) introduced in Eq.(2.29) and the Hamiltonian \( \frac{1}{8\alpha^2} (|p|^2 - 2E)^2 |r|^2 \) introduced in Eq.(2.33) are canonically related. Already in subsection 2.1. we mentioned that the stereographic projection is a conformal mapping transformation. It can be proven that for dimensionality greater than 2 the most general conformal transformation in \( \mathbb{R}^n \) is made out of sphere inversions, euclidean motions and scale transformations [53]. Following [51] we perform the inversion of coordinates

\[ (x')^i = \frac{x^i}{|x|^2}, \]  

(2.34)
so that the corresponding canonical momenta $p'_i = \left( \frac{\partial x^j}{\partial (x')^j} \right) p_j$ become
\[
p'_i = |x|^2 p_i - 2x'(x \cdot p).
\]

It can be checked explicitly that just described transformations are canonical. Next, one should perform the additional (scale) canonical transformation
\[
\bar{x}^i = \frac{p'_i}{b}, \quad \bar{p}_i = -b (x')^i
\]
where $b > 0$ is an adjustable parameter. With these conformal transformations and by adjusting the value of the parameter $b$, the Hamiltonian $\frac{1}{8\alpha^2} (|p|^2 - 2E)^2 |r|^2$, $E < 0$, $|E| = A$, is converted into Hamiltonian, Eq. (2.29), for the fish-eye potential. Quantization of the Schrödinger equation with such potential is discussed in detail in section 4. Additional independent information is provided in Appendix F.

3. Known and unknown roles of conformal invariance in quantum mechanical problems involving fish-eye potentials

3.1. General arguments

In two dimensions using conformal transformations we obtained Eq. (2.21) for the refractive index. Adopted to two dimensions, Schrödinger’s Eq. (2.14a) can be rewritten now as
\[
- \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi - V(x, y) \psi = 0.
\]

In such a form this equation was studied by Makowski [54] for the fish-eye and related potentials. By performing conformal transformation on Eq. (3.1a) and using Eq. (2.21), Eq. (3.1a) can be rewritten in equivalent form as follows
\[
- |f_z(z)|^2 \left( \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2} \right) \psi - |f_z(z)|^2 U(\xi, \eta) \psi = 0
\]
causing the conformal factor $|f_z(z)|^2$ to drop out. Such an omission of the conformal factor is possible because the 2 dimensional Laplacian is conformally invariant. In dimensions higher than two this is no longer true [55]. Thus, beginning with the two-dimensional version of the fish-eye potential and by applying the conformal transformations to this potential, e.g. to Eq. (2.22), and to the Laplacian, Makowski studied the Schrödinger-type equations for a large class of fish-eye-type potentials [54]. Other authors, e.g. see [7-9],[17],[50] used the

\[\text{Actually, the Sturmian-type.}\]
3-dimensional version of the generalized fish-eye potential, Eq.(2.23)\textsuperscript{15} in the corresponding 3-dimensional Schrödinger-type equations without any concern about the mathematical correctness of these equations. By ignoring the issue of conformal invariance, these authors had lost some fundamentally important physics essential not only for solution of the Löwdin problem in atomic physics but, more broadly, for solution of dynamical problems in non flat Bertrand spaces. The role of Lie sphere and conformal geometry in finding the solution of Schrödinger, Klein-Gordon and other wave equations was discussed in detail in our previous work [3]. In this section we are going to add some new details to the topic of conformal invariance by making the unexpected connections between results of section 2 and our previous work [3].

3.2. Important connections between the dynamical time changes and conformal invariance in quantum mechanics, quantum field theory and gravity

In this section we connect the results of Ref.[56]\textsuperscript{16} with those discussed in section 2 and Appendices A and B. We begin with the Lagrangian

\[ L(t, q_i, \dot{q}_i) = \frac{1}{2} g_{ij} \dot{q}_i \dot{q}_j - V(q_i) \] (3.2)

and define the conformal transformation

\[ \tilde{g}_{ij}(q_i) = \omega^2(q_i) g_{ij}(q_i), \] (3.3)

where \( \omega^2(q_i) \) is some positive function of coordinates \( \{q_i\} \). Instead of previously used \( \frac{dt}{d\tau} = \dot{q}_0 \) we write now

\[ d\tau = \omega^2(q_i) dt. \] (3.4)

In view of this result the action

\[ S = \int dt L(t, q_i, \dot{q}_i) \] (3.5a)

should be rewritten now as

\[ S = \int \frac{d\tau}{\omega^2(x)} \left[ \frac{1}{2} \omega^4(q_i) g_{ij} \dot{q}_i \dot{q}_j - V(q_i) \right], \quad q_i' = \frac{dq_i}{d\tau}, \quad q''_i = g^{ij} q'_j, \] (3.5b)

or, equivalently,

\[ S = \int d\tau \tilde{L}(t, q_i, q'_i) \] (3.5c)

where \( \tilde{g}_{ij} = \tilde{g}_{ij}(q) \) is defined by Eq.(3.3) and \( \tilde{V}(\{q_i\}) = \frac{V(\{q_i\})}{\omega^2(q_i)} \). In Appendix B we demonstrated that the Euler-Lagrange equation of motion for \( L(t, q_i, \dot{q}_i) \) and \( \tilde{L}(t, q_i, q'_i) \) produce the

\textsuperscript{15}For \( \gamma = 1/2 \) in [7-9],[17] and for arbitrary \( \gamma > 1 \) in [50]. In view of scaling analysis of Eq.(2.14), arbitrary \( \gamma \)'s are not physically realizable though.

\textsuperscript{16}This paper is containing many typos causing us to rewrite needed equations.
same trajectories. It is of interest to reobtain this result now for a reason which will become clear upon reading.

For \( L(t, q_i, \dot{q}_i) \) the Euler-Lagrange equations are

\[
\ddot{q}^i + \Gamma^i_{jk} \dot{q}^j \dot{q}^k + V,^i = 0
\] (3.6)

while for \( \bar{L}(t, q_i, q'_i) \) these equation acquire the following form

\[
\dddot{q}^i + \hat{\Gamma}^i_{jk} \dot{q}^j \dot{q}^k + \frac{V,^i}{\omega^4(q_i)} - \frac{2V'}{\omega^5(q_i)} \omega(q_i)^i = 0.
\] (3.7)

Here, according to [53], we have for the Christoffel symbols \( \Gamma^i_{jk} \) the following transformation law:

\[
\hat{\Gamma}^i_{jk} = \Gamma^i_{jk} + \delta^i_j (\ln \omega)_k + \delta^i_k (\ln \omega)_j - g_{jk} (\ln \omega)^i.
\] (3.8)

Since

\[
q'^i = \frac{dq^i}{dt} \equiv \ddot{q}^i \frac{1}{\omega^2(q_i)}
\] (3.9a)

and

\[
q''^i = \frac{1}{\omega^4(q_i)} [\dddot{q}^i - 2\dot{q}^i \dot{q}^j (\ln \omega)_j],
\] (3.9b)

by replacing in Eq.(3.7) \( q''^i \) and \( q'^i \) by Eq.s(3.9b) and (3.9a) and using Eq.(3.8) we finally obtain after some algebra

\[
\dddot{q}^i + \Gamma^i_{jk} \dot{q}^j \dot{q}^k + V,^i - 2(\ln \omega)^i (\frac{1}{2} g_{ij} \dot{q}^i \dot{q}^j + V(\{q_i\})) = 0.
\] (3.10)

Here

\[
\frac{1}{2} g_{ij} \dot{q}^i \dot{q}^j + V(\{q_i\}) = E
\] (3.11)

is an energy. By reversing arguments we also obtain the equations of motion for primed variables as well as the analog of \( E \) rewritten in primed variables. Thus, we just obtained the

**Theorem 3.1.** Two dynamical systems are conformally invariant at the level of their respective equations of motion if and only if they both have vanishing total energies.

**Corollary 3.2.** From results of Appendix B it follows that the dynamics of Reeb vector fields is conformally invariant. It is describing the motion on geodesics.

**Corollary 3.3.** Conformal invariance is result of time changing transformations. They make time a canonical variable with energy/Hamiltonian being its conjugate. Use of such transformations brings the Newtonian mechanics into covariant form used for description of dynamics of general relativity. More on this is presented in section 5 in connection with the description of Eisenhart lift and Bertrand spaces.
Extension of these results to nonquantized field theories proceeds analogously. Some representative examples are discussed in [56]. The question arises: How just obtained results can be transferred to quantum mechanics/quantum field theories? In 2 dimensions Eq.(3.1b) demonstrates that this is indeed possible in the case of nonrelativistic quantum mechanics. Therefore, we would like now to demonstrate that since the Theorem 3.1 holds in higher dimensional spaces as well, there should be an analog of this theorem in quantum mechanics/quantum field theories in higher dimensions.

3.3. Treatment of conformal invariance in quantum mechanics and quantum field theory in dimensions higher than two

At the classical level we just discussed conformally related mechanical systems in the previous subsection. If we would follow standard textbooks on quantum mechanics and replace the classical kinetic energy term by the term involving the Laplacian (perhaps defined on the curved space) we would not get the correct answer for conformally related quantum analogs of conformally related classical systems. This is so because the Laplacian is not going to remain form-invariant under conformal transformations. Instead, the conformal (Yamabe) Laplacian \( \Box_g \) must be used. It is defined as follows

\[
\Box_g = -\Delta_g + \alpha(d)R(g),
\]

(3.12a)

where \( \alpha(d) = \frac{d-2}{4(d-1)} \) and \( R(g) \) is the scalar curvature of \( d \)-dimensional Riemannian manifold \( \mathcal{M}_d \) whose metric tensor is \( g_{ij} \). In the case when the Laplacian \( \Delta_g \) is acting on scalar function \( \psi \) its action is defined as [59]:

\[
\Delta_g \psi = g^{ij} \left[ \frac{\partial^2 \psi}{\partial x^i \partial x^j} - \Gamma^k_{ij} \frac{\partial \psi}{\partial x^k} \right].
\]

(3.12b)

Under the conformal change of metric \( \tilde{g} = g \exp(2f) \) the conformal Laplacian is transforming as follows

\[
\Box_{\tilde{g}} = e^{-\left(\frac{d+1}{2}\right)f} \Box_g e^{\left(\frac{d-1}{2}\right)f}.
\]

(3.13)

Ovsyannikov [60] and Ibragimov [61] considered in detail the solutions of partial differential equations of the following type

\[
F[u] = g^{ij} u_{ij} + b^i u_i + cu = 0.
\]

(3.14)

Here \( u_i = \frac{\partial u}{\partial x_i} \), \( u_{ij} = \frac{\partial^2 u}{\partial x_i \partial x_j} \), \( g^{ij}, b^i \) and \( c \) are the known functions of \( x_i \), and \( g^{ij} = g^{ji} \).

Following ideas of Hadamard discussed in our previous work [3], Ibragimov [61], using work by Ovsyannikov [60], demonstrated that for spaces of Riemannian signature use of Hadamard-type transformations of the type discussed in [3] converts Eq.(3.14) into conformally invariant equation

\[
\Box_g \Psi = 0.
\]

(3.15)

\[\text{For a quick introduction to this topic we refer our readers to our works [57,58].}\]
In spaces of Lorentzian signature it is known as well, e.g. read Appendix B of [3] and [61], section 12.2, Lemma 1., that the wave equation

\[ \Box u \equiv \left( \frac{\partial^2}{\partial t^2} - \Delta \right) u = 0 \] (3.16)

adapted for spaces of Lorentzian signature having the pp-type metric (the Penrose limit metric) is conformally invariant and obeys the Huygens principle. Thus, in spaces with pp metrics the conformal invariance is inseparably linked with the Huygens principle [55,61] for such an equation. In [61] it is demonstrated that equations of the type

\[ \Box u + b^i u_i + cu = 0 \] (3.17)

with help of the Hadamard-like transformations are reducible to the standard wave equation

\[ \Box \Phi = 0. \] (3.18)

This property is identical with that for Eq.(3.17) obeying Huygens’ principle. These results are summarized in the following

**Corollary 3.4.** In spaces of Riemannian and pseudo Riemannian signature Eqs.3.14 and, respectively, (3.17) are conformally invariant. For spaces of Lorentzian signature the conformal invariance is inseparably linked with the validity of Huygens’ principle. These equations are quantum analogs of the conformally invariant dynamical equations of classical mechanics discussed in previous subsection.

3.4. Further ramifications

The 3 dimensional analog of 2-dimensional Schrödinger’s Eq.(3.1a) reads as follows

\[- \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi + V(x,y,z)\psi = 0. \] (3.19a)

Here, in view of Eq.(2.23), the potential \( V(x,y,z) \) is given by

\[ V(x,y,z) = - \left( \frac{a}{r} \right)^2 \left[ \frac{n_0}{(r/a)^{-\gamma} + (r/a)^{\gamma}} \right]^2, r^2 = x^2 + y^2 + z^2, a = \text{const.} \] (3.19b)

The quantum mechanical eigenvalue (Sturmian) problem for Eq.(3.19a) with such a potential was formally solved in the foundational work Ref.[7]. Details were further elaborated in [50] for any \( \gamma \). The case \( \gamma = 1 \) corresponds to the Maxwell’s fish-eye potential (and, hence, to the hydrogen atom) while the \( \gamma = 1/2 \) case corresponds to the D-O potential used by these authors for description of electronic structure of the whole periodic system of elements. Corollary 3.4. guarantees that for any \( \gamma \) these equations are conformally equivalent to each

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\(^{18}\)Here \( \Delta \) is flat Laplacian
other. But in section 2 we found that Eq.s(2.14a) and (2.14b) make sense physically only for $\gamma = 1$ or $1/2$.

Given these facts, two questions arise: a) If these Eq.s(3.19) are conformally equivalent, which one of these should be considered as the seed from which others are being obtained? b) What makes Maxwell’s fish-eye ($\gamma = 1$) and D-O ($\gamma = 1/2$) potentials so special if, in fact, they are conformally equivalent? To answer a) we have to remind to our readers some general facts about the conformally related spaces. We begin with

**Definition 3.5.** The (pseudo) Riemannian space $\mathcal{M}_d$ of dimension $d$ is flat if in some region around any point $x \in \mathcal{M}_d$ there is a metric-preferred coordinate system such that

$$ds^2 = g_{ij}(x)dx^i dx^j$$

(3.20)

in which the metric tensor $g_{ij}(x) = e_i \delta_{ij}, e_i = \pm 1$.

**Definition 3.6.** A (pseudo) Riemannian space $\mathcal{M}_d$ is called conformally flat if it can be obtained from the flat space via conformal change of metric tensor according to Eq.(3.3), that is with help of transformation $\bar{g}_{ij}(x) = \omega^2(x)g_{ij}(x)$ with $g_{ij}(x)$ defined in Eq.(3.20).

**Definition 37.** When $\omega^2(x) = \text{const}$, the above conformal transformation is called homothety (or similarity), when $\omega^2(x) = 1$ the homothety is isometry. The isometric-type of motion on $\mathcal{M}_d$ is described in terms of Killing’s equations. The Killing vectors $X$ are solutions of Killing’s equations

$$\mathcal{L}_X g_{ij} = 0,$$

(3.21)

where the Lie derivative $\mathcal{L}_X$ is defined in Eq.(B.5).

**Definition 3.8.** The conformal type of motion on $\mathcal{M}_d$ is described in terms of the conformal Killing equations

$$\mathcal{L}_X g_{ij} = 2\Phi(x)g_{ij}$$

(3.22a)

in which $X$ is the conformal Killing vector [62].

Consider now two conformally related spaces, e.g. let $\bar{g}_{ij}(x) = e^{2\sigma(x)}g_{ij}(x)$. It is of interest to study the relationship between Eq.(3.22a) and

$$\mathcal{L}_X \bar{g}_{ij} = 2\Phi(x)\bar{g}_{ij}.$$  

(3.22b)

It can be demonstrated [61] that

$$\tilde{\Phi}(x) = \Phi(x) + 2\xi^i \frac{\partial \sigma}{\partial x^i}.$$  

(3.23)

Here the (Killing) vector $\xi^i$ is defined by Eq.s (C.2),(C.3) in Appendix C. Eq.(3.23) reminds us about the analogous cases in gauge theories associated with choices of gauges. In particular,
the choice $\Phi(x) = 0$ implies that the underlying space with the metric $\bar{g}_{ij}$ is completely rigid. It admits only isometric (non bendable/ non stretchable) motions. Although physically non realistic, such spaces do exist mathematically [61] and can be constructed based on the equation

$$\Phi(x) + 2\xi^i \frac{\partial\sigma}{\partial x^i} = 0.$$  

(3.24)

These spaces are serving as boundaries of conformally flexible/bendable spaces or can occur as subspaces of these spaces. In Appendix C we established that for the Riemannian spaces $M_d$ of dimensionality $d$ the isometric motion is described in terms of the (maximum) $\frac{d(d+1)}{2}$ parameters. The maximum is achieved for spaces of constant curvature. The question arises: What is the maximal number of parameters required for description of conformally related spaces?

To answer this question, we have to extend the analysis presented in Appendix C. In particular, we have to count $d$ Killing vectors $\xi^i$ as well as the factor $\Phi$. Altogether there are $d+1$ such terms. In addition, however, we should account for $d^2$ terms like $\nabla_k \xi^i$ and $d$ terms like $\partial_k \Phi$. Their role is nicely explained in [63], section 1. Thus, altogether we obtain: $d^2 + d + d + 1 = (d+1)^2$ parameters. The truly nontrivial conformal motion is described in terms of $(d+1)^2 - \frac{d(d+1)}{2} = \frac{1}{2}(d+1)(d+2)$ parameters. In [61] there is a proof of the following remarkable

Theorem 3.9. (Pseudo) Riemannian space $M_d$ has nontrivial conformal group of motions only if $M_d$ is conformally equivalent to the conformally flat space.

Definition 3.10. The conformal group is trivial if use of the relation $\bar{g}_{ij}(x) = \omega^2(x)g_{ij}(x)$ leads to Eq.(3.24) possessing a nonzero solution.

Corollary 3.11. According to Theorem C.1. The maximum number of parameters $\frac{d(d+1)}{2}$ is possible only for spaces $M_d$ of full isometry group which are of constant scalar curvature. But, according to Corollary C.3., all spaces of constant scalar curvature are conformally flat. This means that such manifolds have exactly $\frac{1}{2}(d+1)(d+2)$ conformal parameters involved in nontrivial conformal group according to Theorem 3.9.

This fact can be illustrated with help of Eq.s(3.12a) and (3.13). Suppose that in Eq.(3.12a) the metric $\bar{g}$ is describing the space of constant scalar curvature. Because such a space is conformally flat we can write

$$e^{-\left(\frac{d}{2}+1\right)f} (-\Delta g=1) e^{\left(\frac{d}{2}-1\right)f} = \Box \bar{g}$$

(3.25)

where $g = 1$ is actually $g = \delta_{ij}$ is the Euclideanized version of the metric defined in Eq.(3.20). Thus, we are having two reference manifolds : a) The manifolds of constant scalar (nonzero)

\footnote{This theorem is compatible with existence of conformally flat Bertrand spaces [18] described in section 5 and Appendix E.}
curvature and b) The manifolds whose scalar curvature is exactly zero. All other conformally flat manifolds whose scalar curvatures are nonconstant can be related (deformed) either to a) or to b)-type of manifolds (these are conformally equivalent, of course). This was the point of departure of Yamabe’s work [64]. An excellent modern exposition of Yamabe ideas is given in [65]. For a rapid introduction to this topic, please, consult our previous works [57] and [58].

Based on just described results, we argue below that the Schrödinger equation for the Maxwell fish-eye potential should be taken as the seed. This will provide us an answer to the question a). Foregoing development makes perfect sense physically since such an equation corresponds to the stationary Schrödinger equation for hydrogen atom. This is demonstrated in detail in section 4 and also below, in this section. It means as well that the equation proposed by D-O (\(\gamma = 1/2\)) for describing the spectra of other multielectron atoms is obtainable as conformal deformation of the Schrödinger equation for the hydrogen atom. Such a deformation is to be described below. It will be also described in the Appendix F from the alternative standpoint. Results are fully compatible with the modified Bertrand theorem (to be discussed in section 5).

3.5. Schrödinger’s equation for hydrogen atom from Ovsyannikov’s work on group-theoretic analysis of differential equations

3.5.1. General facts

Here by Schrödinger’s equation for hydrogen atom we mean Eq.(3.19a) with the potential defined by Eq.(3.19b) (where we have to put \(\gamma = 1\)). At the classical level the fish-eye-Coulomb problem equivalence was demonstrated in section 2. At the quantum level it is demonstrated in section 4.

Obviously, we are not going to copy and paste Ovsyannikov’s results [60] in this subsection since Ovsyannikov’s book does not have physical or chemical applications in it. One of the purposes of this subsection is to develop such applications. In doing so, we shall mainly use the Chapter 8 of [60]. Incidentally, it begins with our Eq.(3.14). Ovsyannikov applies to this equation three types of Hadamard-type transformations. These are exactly the same as discussed in our work [3] culminating there in Theorem 4.1. Unlike [3], such transformations are to be described in much greater detail now with the purpose of transforming Eq.(3.14) into the D-O form, Eq.(3.19) (firstly with with \(\gamma = 1\)) By working out this transformation in detail will demonstrate to our readers that use of the same type of transformations is transforming Eq.(3.14) into Eq.(3.19) with any preassigned \(\gamma\) factor.

\[\text{21}\] We are grateful to the staff members of the Department of Mathematics of the Novosibirsk State University for supplying us with the original (Russian) version of Ovsyannikov’s notes subsequently converted into a book. They contain many details omitted upon conversion of the notes into a book and translation of Ovsyannikov’s book into English.
In compliance with Hadamard method summarized in Theorem 4.1. of [3], we consider now the 3 types of Hadamard transformations in full generality.

(α) The coordinate transformation

\[ x'^i = p^i(x), \quad i = 1, \ldots, d. \]  

(3.26a)

It leads to \( u = u' \circ p \) implying

\[ F'\left[u'\right] = g^{i\bar{j}} u'_{i\bar{j}} + b^i u'_i + c' u' = 0. \]  

(3.26b)

In this equation \( u'_i = \frac{\partial}{\partial x'_i} u' \), etc., \( g^{k\bar{l}} \circ p = g^{i\bar{j}} p^k_i p^l_j, b^k \circ p = g^{i\bar{j}} p^k_i + b^i p^k_i, c' \circ p = c, p^k_i = \frac{\partial}{\partial x'_i} b^k \), etc.

(β) The scale transformation

\[ F'\left[u\right] = e^{-\theta} F\left[e^\theta u\right] \]  

(3.27a)

It is converting Eq.(3.14) into

\[ F'\left[u\right] = g^{i\bar{j}} u_{i\bar{j}} + b^i u_i + c u = 0 \]  

(3.27b)

Here \( b^i = b^i + 2g^{i\bar{j}} \theta_{\bar{j}} \) and \( c' = c + b^i \theta_i + g^{i\bar{j}} \theta_{i\bar{j}} + g^{i\bar{j}} \theta_{ij} \).

(γ) The conformal transformation

\[ F'\left[u\right] = e^{-2\theta} F\left[u\right]. \]  

(3.28a)

It results in

\[ F'\left[u\right] = \tilde{g}^{i\bar{j}} u_{i\bar{j}} + \tilde{b}^i u_i + \tilde{c} u = 0. \]  

(3.28b)

Here \( g^{ij} = e^{2\theta} \tilde{g}^{ij}, b^i = e^{2\theta} \tilde{b}^i \) and \( c = e^{2\theta} \tilde{c} \).

Transformations (α) and (β) leave Eq.(3.14) in the same (pseudo) Riemannian space \( \mathcal{M}_d \). The transformation (γ) conformally relates \( \mathcal{M}_d \) to \( \tilde{\mathcal{M}}_d \).

These statements require proofs. We shall not reproduce these proofs referring our readers to Ovsyannikov’s book [60]. Nevertheless, results of these proofs cause us to introduce the scalar \( H \) and the tensor \( K_{ij} \) to be defined momentarily. For this purpose, following Ovsyannikov [60], we have to define the contravariant vector \( a^i \) via

\[ a^i = b^i \pm g^{kl} \Gamma^i_{kl}, \quad i = 1, \ldots, d. \]  

(3.29a)

Ovsyannikov uses only sign ”+” in his calculations but below we shall argue that, in fact, both signs should be used. Since under (α)—type of transformations Christoffel’s symbols transform as

\[ \Gamma^k_{ij} p^l_i = p^k_l + \Gamma^k_{im} p^m_i p^l_j, \]  

(3.30)

it can be demonstrated that the contravariant vector \( a^i \) obeys the standard rule of transformation for vectors:

\[ a'^k = b'^k \pm g^{ml} \Gamma^k_{ml} = (b^i \pm g^{kl} \Gamma^i_{kl}) p^k_i = a^i p^k_i. \]  

(3.29b)
With help of such defined vector $a^i$ it becomes possible to introduce a skew-symmetric tensor $K_{ij}$ via

$$K_{ij} = a_{i,j} - a_{j,i}, \quad (3.31)$$

where $a_{i,j} = \frac{\partial a_i}{\partial x^j} - a_i \Gamma^l_{ij}$ and the raising and lowering of indices is made with help of the metric tensor $g_{ij}$, as usual. Accordingly, the scalar $H$ can now be defined as

$$H = -2c + a^i_{,i} + \frac{1}{2}a^i a_i + 2\alpha(d)R(g). \quad (3.32)$$

Thus defined $H$ and $K_{ij}$ allow to prove the following

**Theorem 3.12.** $H$ and $K_{ij}$ remain unchanged under transformations of $(\beta)$—type converting Eq.(3.14) into Eq.(3.27b). They are the invariants of $(\beta)$—type transformations.

It can be also proven that with respect to transformations $(\gamma)$ the tensor $K_{ij}$ will remain unchanged. So it is also an invariant of $(\gamma)$—type transformations. At the same time, the scalar $H$ is transformed into $\tilde{H} = e^{-2\theta}H$. Therefore, it looses its invariance property. The conformal Killing Eq.s(3.22a) can be rewritten in a more familiar form now as

$$\nabla_i \xi_j + \nabla_j \xi_i = \mu g_{ij}, \quad \mu = 2\Phi. \quad (3.33)$$

With help of these equations, it also can be demonstrated that

$$\xi^k H_{,k} + \mu H = 0. \quad (3.34a)$$

If $H \neq 0$, it can be demonstrated as well that it is always possible to select $\theta$ in Eq.(3.28a) so that $H = e^{2\theta}$. Such a selection leads to $\tilde{H} = 1$. In such a case, the transformed equation

$$\xi^k \tilde{H}_{,k} + \tilde{\mu} \tilde{H} = 0 \quad (3.34b)$$

is implying that $\tilde{\mu} = 0$. Therefore, whenever $H = e^{2\theta}$, we are back to the Killing Eq.s (C.4) implying that we are dealing with the isometry subgroup containing $\frac{(d+1)d}{2}$ generators inside larger nontrivial conformal group. This fact is in accord with Yamabe’s ideas [64] that ”more flexible” spaces $\mathcal{M}_d$ are conformally deformable into spaces of constant scalar curvature.

To make a progress, from now on we shall deal only with the conformally flat metric, that is with the metric of the type $g^{ij}(x) = \rho(x)\delta^{ij}$ or with $g_{ij}(x) = \frac{1}{\rho(x)}\delta_{ij}$. To illustrate the value of just described results, we begin with the simplest but instructive example.

### 3.5.2. Geometrical meaning of the stationary Schrödinger’s equation for hydrogen atom

Instead of considering Eq.(3.14), we shall focus now on Schrödinger’s Eq.(3.19a) written in the form

$$\rho \Delta u + cu = 0 \quad (3.35)$$
in which we initially do not require \( c(x) \) to be a constant and use the notation \( \Delta = \Delta_{g=1} \) as before. This equation plays a significant role also in section 5.

By looking at Eq.(3.27b) and comparing it with Eq.(3.14), we realize that in Eq.(3.35) \( b' = 0 \) and \( c \) in this equation should be actually relabelled as \( c' \). By looking at Eq.(3.29b) and by noticing that for the \((\beta)\)-type transformations \( g_{ij} = g'^{ij} \) causing \( \Gamma^k_{mi} = \Gamma^i_{kl} \), the combination \( g_{kl} \Gamma^i_{ki} = \frac{d-2}{2} \frac{\partial}{\partial x^i} \ln \rho \). This result is obtained in the Appendix D. From Eq.(3.29b) we obtain

\[
\alpha_i' = \pm \frac{d-2}{2} \frac{\rho_j}{\rho} \text{ or } \alpha_i'' = \pm \frac{d-2}{2} \delta_{ij} \frac{\rho_i \rho_j}{\rho}.
\]

(3.36)

In view of Eq.(3.32) we have to calculate

\[
\alpha_i'' = \frac{\partial \alpha_i''}{\partial x^i} + \alpha_k \Gamma^i_{ki} = \pm \left( \frac{d-2}{2} \delta_{ij} \rho_i \rho_j - \frac{d(d-2)}{4} \delta_{ij} \frac{\rho_i \rho_j}{\rho} \right),
\]

(3.37)

where we used Eq.(D.8) of the Appendix D for calculation of \( \Gamma^i_{ki} \). Besides,

\[
\frac{1}{2} a'' a_i' = \frac{(d-2)^2}{8} \delta_{ij} \rho_i \rho_j.
\]

(3.38)

In view of Eq.(3.32), by combining Eq.s(3.37) and (3.38) we obtain,

\[
a_i'' + \frac{1}{2} a'' a_i' = \frac{(d-2)^2}{8} \delta_{ij} \rho_i \rho_j - \frac{d^2 - 4}{4} \delta_{ij} \frac{\rho_i \rho_j}{\rho}.
\]

(3.39)

Calculating this result we selected the sign "+" in Eq.(3.36). This is caused by the following considerations. For spaces of constant curvature the conformal factor \( \rho \) was obtained in Appendix C. By adopting the Euclidean version of the metric given in Eq.(C.7), small calculation using Eq.s(3.36),(3.37) results in

\[
a_i'' + \frac{1}{2} a'' a_i' = \frac{d(d-2)}{2} K.
\]

(3.40)

Going back to Eq.(3.32) and taking into account that \( \frac{d-2}{2(d-1)} = 2\alpha(d) \) and that, according to [66], for spaces of constant scalar curvature \( R(g) = -d(d-1)K \), we obtain \( 2\alpha(d)R(g) = - \frac{d^2}{2} K \). By combining this result with Eq.(3.40) and using it in Eq.(3.32) we obtain:

\[
H' = -2c' + a_i'' + \frac{1}{2} a'' a_i' + 2\alpha(d)R(g) = -2c'.
\]

(3.41)

But since \( H \) is invariant of \((\beta)\)-transformations, by construction, we must have \( H' = H \). In view of Eq.(3.41), this is only possible when \( c' \) is a constant. In such a case Eq.(3.35) is the stationary Schrödinger’s equation for the hydrogen atom according to Eq.s(3.19a) and (3.19b) where we have to select \( \gamma = 1 \).

3.5.3. Conformal (Yamabe) Laplacian equation treated by Hadamard-Ovsyannikov
Using Eq.s(3.12a) and (3.12b) we consider now the following equation

\[ F[u] = \Box_g u = -\rho \partial^i u_i + \frac{d-2}{2} \rho^i u_i + \alpha(d) R(\rho) u = 0. \]  

(3.42)

Clearly, it is of exactly the same type as Eq.(3.14). Therefore, in Eq.(3.42) we must have \( b^i = -\frac{d-2}{2} \rho^i, \) \( c = -\alpha(d) R(\rho) \). At first, we consider this equation for the space of constant scalar curvature. From previous subsection we know that in such a case \( 2 \alpha(d) R(g) = -\frac{d(d-2)}{2} K \). Using this result we can replace the term \( c = -\alpha(d) R(\rho) \) by \( c = \frac{d(d-2)}{4} K \). Now we want to compare Eq.(3.42) with Eq.(3.35) since they both have the same \( \rho \) factor. Recall that the \((\beta)-type \) transformations do not change the metric of underlying space. Since this is so, the equality of invariants \( H = H' \) leads to the result:

\[ a^i + \frac{1}{2} a^i a_i = -2c' + d(d-2) K = \text{const}. \]  

(3.43)

To check this result we notice that the contravariant vector \( a^i \) is defined by Eq.(3.29a). The term \( g^{kl} \Gamma^i_{kl} \) in this equation is calculated in the Appendix D, Eq.(D.2). Therefore, by selecting the “+” sign we obtain,

\[ a^i = b^i + g^{kl} \Gamma^i_{kl} = -\frac{d-2}{2} \rho^i + \frac{d-2}{2} \rho^i = 0, \]  

(3.44)

implying \( c' = \frac{d(d-2)}{2} K \). Thus, \( c' = 2c \) which makes physical sense. Notice, in arriving at this result Eq.(3.44) was used in which we have not made any specification of the conformal factor. The result \( a^i = 0 \) was obtained by Ibragimov [61], page120, by different set of arguments.

Just obtained result gives us an opportunity to take also a look at the Yamabe Laplacian for the metric other than that of constant scalar curvature. To do so we put the factor \( \psi \) in Eq.(D.7) temporarily to zero in view of Eq.(3.44). Then, in view of Eq.s (3.13),(3.27a), we write \( e^\theta = (e^{2f})^{d-2} \). To utilize fully Eq.(3.13) we have to use Eq.(3.28a), that is we have to use the \((\gamma)\) transformation which is connecting equations with conformally related metrics. To facilitate matters, we notice that the combination \( e^{2f} e^{-\theta} F[e^\theta u] \) in which \( e^\theta = (e^{2f})^{d-2} \) produces exactly the same result \( e^{-\lambda(x)} f F[e^{(d-1)/2} u] \) as was recorded already in Eq.(3.13) for the Yamabe Laplacian. This provides us with an independent check of correctness of our computations since the conformal factor \( e^{2f} \) is present in the equation \( \bar{g}_{ij}(x) = e^{2f(x)} g_{ij}(x) \) defining conformally related spaces. We still have to comment on several topics.

3.6. Miscellaneous

First, we need to comment on the role of \((\alpha)\)-transformations. Such type of transformations are described in detail in the monumental work, [67], Chapter 3. These are needed to
bring the PDE’s, Eq. (3.14), into the canonical/standard form. Also these transformations had been used for defining the contravariant vector $a^i$. Since we are using only the metric of the type $g^{ij}(x) = \rho(x)\delta^{ij}$, this spares us from the necessity to consider ($\alpha$) transformations further.

Second, in using the ($\beta$)-type transformations we are replacing the coefficients $b^i$ and $c$ by $b'^i$ and $c'$ using the same factor $\theta$. This means that by properly selecting $\theta$ we can always replace the factor $c$ by the pre assigned factor $c'$. However, in such a case the factor $b^i$ cannot be forced to become zero. For this to happen, in addition to parameter $\theta$, the parameter $\psi$ defined in Eq.(D.5) should be used. If we would select the sign “-” initially in Eq.(3.29a), the result $a^i = 0$ in Eq.(3.44) will change into

$$a^i = -(d-2)\rho^i.$$  

This is helpful if we want to use Eq.s(D.3)-(D.7) from Appendix D. These equations should be used as follows.

a) Using the equation $c' = c + b^i\theta_i + g^{ij}\theta_j + g^{ij}\theta_i\theta_j$ with pre assigned $c'$ factor we can determine the factor $\theta$. For this purpose we need to solve the PDE equation $g^{ij}\theta_{ij} + g^{ij}\theta_i\theta_j + b^i\theta_i = c' - c$. Its solution is greatly facilitated by our use of spherical symmetry.

b) Use of this result in Eq.(D.7) determines the factor $\psi$.

c) After these two factors are determined, equations $b'^i = b^i + 2g^{ij}\theta_j$ and $c' = c + b^i\theta_i + g^{ij}\theta_j + g^{ij}\theta_i\theta_j$ yield one-to one relations between $c'$ and $c$ and $b'^i$ and $b^i$ in such a way that we can put $b'^i = 0$.

In treating the hydrogen atom case in subsection 3.5.2 to keep $b'^i = 0$ is essential. The hydrogen atom case was treated based on Eq.(3.19) where we had selected $\gamma = 1$. But for $\gamma \neq 1$ the same equation can also be brought into canonical form

$$\rho\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)u + c'u = 0 \quad (3.46a)$$

in which

$$\rho = \left[\tilde{V}(x,y,z)\right]^{-1}, \quad c' = \text{const}. \quad (3.46b)$$

In such a form it is used in section 5. Eq.(3.35) is our physical analog of Eq.(3.27b). In Eq.(3.27b), we have: $\rho = [V(x,y,z)]^{-1}$, $b'^i = 0$ and $c' = \text{const}$. Next, we use Eq.(3.42) which is an analog of Eq.(3.14). In it, we use the $\rho-$ factor just defined. Further, in this equation we have $b'^i = -\frac{d-2}{2}\rho i$ and $c = -\alpha(d)R(\rho)$, as required. Now, we need to relate Eq.(3.42) with Eq.(3.46a) using ($\beta$)-type transformations. This is achievable as we just described above. Next, by inverting these operations and using transformation described in Eq.(3.13) we conformally relate the D-O Eq.(3.46a) describing the multielectron atoms with Eq.(3.35) describing the hydrogen atom. To answer the question b) posed in subsection 3.4., we follow analysis made by Ovsyannikov [60] in Chr.8, section 10. In it he considers the Lie algebras of two versions of Eq.(3.46a). One- with $\rho \neq 1$ and, another-with $\rho = 1$. In the last case the Lie algebra is made of two types of generators: a) translations: $\frac{\partial}{\partial x_i}$, and, b) rotations $x^i\partial_j - x^j\partial_i$. While in the first case it is made of the same translations as in the second, but the rotation
generators change now into \((2x_i x^k + (1 - \rho^2)\delta^k_i)\partial_k - (d - 2)x_i u\partial_u, \ i = 1, \ldots, d\). These two sets of Lie algebras cannot be smoothly converted into each other. Only the Lie algebra for Eq.(3.46a) with \(\rho \neq 1\) makes physical sense. It conformally relates the metric of constant scalar curvature (the hydrogen atom case) with the modified metric induced by the presence of the rest of electrons. The reminder of the Part I and the whole Part II are devoted to ramifications of this statement.

4. From analysis to synthesis

4.1. General remarks

Already in their first seminal work [7], Demkov and Ostrovsky discussed method of solving Eq.s(3.19a),(3.19b) in full generality. Subsequently, their results were further developed in [8, 17, 50, 68], etc. These papers differ from each other by the extent of generality of employing the potential, Eq.(3.19b), in Eq.(3.19a). In this section we shall entirely reconsider all these results since none of them is without mistakes. One of the purposes of this section is to correct these mistakes. As a by product new quantum mechanical formalism of dealing with discrete spectrum of hydrogen and many electron atoms is developed. It is tested on known examples and, subsequently, it is extended along directions outlined in [7]. While doing so, we shall connect results obtained in section 3 with those to be presented in this section. We begin with the following observation.

4.2. Basics of R-separation and superintegrability. Relation to Bertrand spaces

The 3-dimensional flat space Laplace equation

\[
\Delta \Psi(x) = 0
\]  

according to [69],[70] admits 11 separable coordinate systems. At the same time, there are 17 coordinate systems for the same Laplace equation permitting R-separation of variables.

**Definition 4.1.** An R-separable coordinate system \(\{u,v,w\}\) for Eq.(4.1) is a coordinate system which permits a family of solutions

\[
\Psi_{\lambda,\mu}(x) = R(u, v, w) U_{\lambda,\mu}(u)V_{\lambda,\mu}(v)W_{\lambda,\mu}(w),
\]

where \(\lambda\) and \(\mu\) are separation constants and \(R\) is a fixed factor such that it is either \(R \equiv 1\) (pure separation) or \(R \neq 1\) and \(R\) cannot then be written in the form \(R = R_1(u)R_2(w)R_3(w)\).

This property of R-separation for the Laplace equation happens to be a general trend. The PDE equations admit more non equivalent R-separable coordinate systems than separable coordinate systems. Here we shall be mainly concerned with the separation options for

\[^{22}\text{E.g. some of the papers discussed only the physically relevant case: } \gamma = 1/2,\text{etc.}\]
the conformal Laplacian, Eq.s(3.12a),(3.15), and its classical Hamilton-Jacobi analog- the equation for the null geodesics
\[ g^{ij} \partial_i W \partial_j W = 0. \] (4.3)

Our interest in conformal (Yamabe) Laplace and null geodesics equations is coming from the results of Appendix B. In it we demonstrated that the Reeb dynamics is always taking place on null geodesics. Quantum mechanically this leads to study of solutions of the conformal (Yamabe) Laplacian equation.

The Eq.(4.3) is additively separable. This means that there is a system of coordinates \( \{ q_i \} \) in which it can be split into a system of ordinary differential equations implying the solution in the form
\[ W = \sum_{i=1}^{d} W(q_i; c_\alpha), c_\alpha \in \mathbb{R}, \alpha = 1, \ldots, d. \] (4.4)

Here \( c_\alpha \) are some known (pre assigned) constants. For the conformal Laplacian and in Eq.(4.3) it is assumed that: a) \( g^{ii} \neq 0 \) and b) \( g^{ij} = 0 \) for \( i \neq j \). This leads to separability in terms of orthogonal coordinates.

Both Eq.s(3.15) and (4.3) are manifestly conformally invariant. Suppose now that \( \Psi \) is R-separable solution of Eq.(3.15), i.e. of equation \( \Box_g \Psi = 0 \). Then, \( e^{-\left(\frac{d}{2}-1\right)f} \Psi = \tilde{\Psi} \) is a also a solution of \( \Box_{\tilde{g}} \tilde{\Psi} = 0 \).

**Corollary 4.2.** If \( \Box_g \Psi = 0 \) possesses an R-separable solution, then \( \Box_{\tilde{g}} \tilde{\Psi} = 0 \) also posses an R-separable solution. Thus, R-separability of the conformal Laplacian is conformally invariant property.

**Corollary 4.3.** The equation \( \Box_g \Psi = 0 \) is R-separable only if the metric \( g \) is conformally flat. A necessary condition for the R-separability of Eq.(3.15) is for the Hamilton-Jacobi equation for the null geodesic, Eq.(4.3), to be additively separable in the same separable coordinates [72].

**Remark 4.4.** Pure separation is a special case of the R-separation. This follows from Eq.(3.25).

**Remark 4.5.** R-separability is tightly linked with the superintegrability. The superintegrability in turn is tightly linked with the fact that for superintegrable systems all dynamical trajectories are closed [72][3]. Superintegrable 2d dimensional dynamical system has more than \( d \) integrals of motion. Those systems which have \( d \) integrals of motion are just integrable. Since for superintegrable systems all dynamical trajectories are closed brings us

\[ ^{23} \text{The latest applications of superintegrability in optics is given, for example, in [73]. Closed geodesics sometimes are called periodic geodesics in mathematical literature [74].} \]
instantly to the problematics of Bertrand spaces [20],[75]. Dynamics in such spaces is super-
integrable by definition. Accordingly, such dynamics admits quantization. Further details on
superintegrability and Bertrand spaces are presented in section 5.

Based on the results of previous section these properties single out Schrödinger’s Eq.(3.19a)
in which we have to put $\gamma = 1$ for the hydrogen atom. Other physically meaningful solutions
are obtainable from that for hydrogen atom with help of conformal transformations by
using Eq.(3.13).

In [7, 8, 17, 50, 68] the spherical symmetry of the potential, Eq.(3.19b) (for any $\gamma$) was
taken into account at the outset leading to the standard protocol of separation of variables
just like that for the hydrogen atom. Unfortunately, all these treatments are mathematically
incorrect. This is explained in detail below, in this section. Nevertheless, the account of
spherical symmetry was done correctly leading to separation of variables. Use of Corollaries
4.2. and 4.3. allows then to obtain different integrable cases from the one (seed) solution,
e.g. that for the hydrogen atom.

4.3. Relationship between the contact geometry, the Eisenhart lift and,
the various types of Stäckel transforms

Relevant fundamentals of contact geometry are described in Appendix B. The essence of
the Eisenhart lift is nicely summarized in [76]. At the level of classical mechanics the Eisen-
hart lift is a method of enlargement of the phase space of dynamical system resulting in the
associated system whose dynamics is taking place on geodesics. Because of this, such a lift
serves as an alternative to the Jacobi- Maupertius formulation of classical dynamics as de-
scribed in Eq.(B.16) of Appendix B. A slight elaboration on Jacobi- Maupertius formulation
of mechanics leads to the equation describing the Reeb dynamics on null geodesics, that is
to Eq.(4.3). From here it follows that use of the Eisenhart lift is facilitating separability and
superintegrability [77]. In the formalism of Eisenhart lift Eq.(4.3) is interpreted as the null
constraint $\mathcal{H} = 0$ imposed on new Hamiltonian $\mathcal{H}$. This constraint is essential for recovery of
the original dynamics from the lifted one [78]. The equation $\mathcal{H} = 0$ coincides with that for the
Reeb vector field as described in Appendix B (after Eq.(B.17)). The additive solution for the
null geodesics, Eq.(4.3), depends on $c_\alpha$ constants defined in Eq.(4.4). As mentioned in the
previous subsection, the additivity of the solution of Eq.(4.3) is essential for the separability
(or R-separability) of the solution of equation $\Box_g \Psi = 0$. Different set of admissible constants
for Eq.(4.3) cause different type of R-separability in Eq.(3.15). It happens that the existence
of separable coordinates has a coordinate-free characterization [79]. This property leads to
the following

Definition 4.6. **Stäckel transform** maps the constants of motion for one orthogonally
separable system to the constants of motion for another orthogonally separable system. Two
systems related by a sequence of Stäckel transforms are **Stäckel-equivalent**.

Remark 4.7. Stäckel equivalence and superintegrability are inseparably linked to each
other [80]. Recently Tsiganov demonstrated [81] how to determine Stäckel matrices preserving superintegrability. Since the number of R-separable coordinates is always finite (for a given dynamical system), the number of Stäckel transforms is also finite. Evidently, none of them changes physics. But all of them are linked with the topology of the underlying manifolds through the issue of closed/periodic geodesics [82]. Although this topic is open for study, references [83], [84] might serve as good starting point for studying this issue.

4.4. Hydrogenic wave functions

4.4.1. A panoramic view

The superintegrability for the Kepler-Coulomb mechanical problem was studied recently in connection with Betrand spaces in [20]. This fact is helpful. It will be further considered in section 5. It cannot be used immediately though for reasons which will become evident upon reading.

It appears, that the topic of solution of the Schrödinger equation for hydrogen atom is so well known that there is nothing which can be added to this subject. This prevailing opinion happens to be incorrect. Indeed, what is taught in any class on quantum mechanics is that the hydrogenic wave functions $\Psi$ are given by the product [85]

$$\Psi_{nlm}(r, \theta, \varphi) = const \rho^l e^{-\frac{r}{2}} L_{n+l}^{2l+1}(\rho) Y_{lm}(\theta, \varphi).$$ (4.5)

Here $\rho = \frac{2r}{n}, n = \sqrt{\frac{1}{2E}}, r$ is the radial coordinate, $E$ is the energy, $E < 0$, $Y_{lm}(\theta, \varphi)$ are the spherical harmonics, $L_{n+l}^{2l+1}(\rho)$ are the generalized Laguerre polynomials. The system of units was chosen in which Bohr’s radius $a_0 = 1$. The constant $\text{const}$ is determined by normalization of the wave function. Since these results are standard, no more details are provided. Much lesser known are four dimensional representations of the hydrogen wave functions taking into account explicitly the hidden O(4) symmetry.\footnote{Surely, the total dynamical symmetry of the hydrogen atom is SO(4,2). This fact is discussed at length in [1] and [3]. Nevertheless, the account of O(4) symmetry is sufficient for now [86]. Once results for the wave functions with O(4) symmetry are known, the SO(4,2) results are easily obtainable with help of the wavefunctions with O(4) symmetry. [1], [87], [88].} According to [87], [89] in 4 dimensions the wave function is looking as follows

$$Y_{nlm}(\alpha, \theta, \varphi) = 2^{l+1} \frac{\Gamma(n-l-1)!}{\Gamma(n)!} \left[ \sin \alpha \right] C_{n-l-1}^{l+1}(\cos \alpha) Y_{lm}(\theta, \varphi).$$ (4.6a)

Here the spherical harmonics $Y_{lm}(\theta, \varphi)$ are the same as in Eq.(4.5) while $C_{n-l-1}^{l+1}(\cos \alpha)$ are the Gegenbauer polynomials to be discussed at length below. Unlike 3 dimensional spherical system of coordinates which is well known, the 4 dimensional system of coordinates

\begin{align*}
x_1 &= r \sin \alpha \sin \theta \cos \varphi, \\
x_2 &= r \sin \alpha \sin \theta \sin \varphi, \\
x_3 &= r \sin \alpha \cos \theta, \\
x_4 &= r \cos \alpha.
\end{align*} (4.7)
is known in standard textbook literature much less. It should be noticed, that already in 3 dimensions there is a number of separable coordinate systems. In addition to spherical, there are cylindrical, parabolic, etc. coordinate systems. These are Stäckel-equivalent and, hence, make the hydrogen atom a superintegrable problem [20]. The choice of coordinate system is dictated by the physics of the problem. In 4 dimensions the number of separable coordinate systems increases remarkably. Many of them are listed in [86]. However, in [89] yet another coordinate system, introduced by Bateman in 1905, is discussed. It will be described in the next section.

In the meantime, the normalization conditions for \( Y_{nlm}(\alpha, \theta, \varphi) \) are

\[
\int_0^\pi \sin^2 \alpha d\alpha \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\varphi \bar{Y}_{n'l'm'} Y_{nlm} = \delta_{n,n'} \delta_{m,m'} \delta_{l,l'}. \tag{4.8}
\]

Interestingly enough, Eqs. (4.5), (4.6) can be compared with each other thanks to the result published as Appendix 5 of the book [91]. By introducing the Fourier transform of \( \Psi_{nlm}(r, \theta, \varphi) \) via

\[
\Phi_{nlm}(p, \theta, \varphi) = (2\pi)^{-\frac{3}{2}} \int d^3r e^{-ip \cdot r} \Psi_{nlm}(r, \theta, \varphi), \tag{4.9}
\]

where we had put \( \hbar = 1 \), after some very detailed calculation described in [91], the final result is looking as follows: \( \Phi_{nlm}(p, \theta, \varphi) = F_{nl}(p) Y_{lm}(\theta, \varphi) \),

\[
F_{nl}(p) = \left[ \frac{2(n-l-1)!}{\pi (n+l)!} \right]^\frac{1}{2} n^{2l+2} l! (np)^l \frac{1}{([np]^2+1) C_{n-l-1}^{l+1}} \frac{1-(np)^2}{1+(np)^2}. \tag{4.10a}
\]

To compare this result with Eq.(4.6a) we need to consult [86], page 649. According to this reference we should get an equality\(^{26}\) if we multiply the 3-dimensional result, Eq.(4.9), by the \( p-\)factor defined by

\[
Y_{nlm}(\alpha, \theta, \varphi) = \frac{p_0^{-1}(p^2 + p_0^2)^2}{4} \Phi_{nlm}(p, \theta, \varphi). \tag{4.10b}
\]

To check the correctness of this proposition, we adopt the spherical coordinates defined by Eq.(4.7) to the case of 3-sphere of unit radius and use the Fock parametrization of this 3-sphere [92]. Specifically, in this parametrization

\[
x_4 = \frac{p_0^2 - p^2}{p_0^2 - p^2} = \frac{1 - (np)^2}{1 + (np)^2} = \cos \alpha. \tag{4.11}
\]

\(\text{E.g. read [90].}\)

\(\text{It should be noted that in [86] the combination } p_0^{-1}(p^2 + p_0^2)^2 \text{ was written as } p_0^{-\frac{5}{2}}(p^2 + p_0^2)^2. \text{ This is caused by the fact that, instead of the constant factor } \left[ \frac{l+1}{2\pi(n+l)!} \right]^\frac{1}{2} \text{ taken from [89] in Eq.(4.6a) the factor } \left[ \frac{l+1}{2\pi(n+l)!} \right]^\frac{1}{2} \text{ was used erroneously.}\)

\(\text{See also Eq.s(2.2),(2.3) in addition.}\)
We also took into account that \( p_0 = \sqrt{-E}, E < 0, -E = 1/n, m = 1/2, \) \( m \) is the electron mass in selected system of units. Based on this information, we obtain:

\[
(n_p)^2 = \frac{1 - \cos \alpha}{1 + \cos \alpha}.
\]  

(4.12)

Next, using this result, we obtain as well:

\[
(n_p)^2 + 1 = \frac{2}{1 + \cos \alpha}, \quad \text{and} \quad \left( \frac{1 - \cos \alpha}{1 + \cos \alpha} \right)^l \left( \frac{1 + \cos \alpha}{2} \right)^{l+2}
\]

and, therefore,

\[
p_0^{-3} \left[ (n_p)^2 + 1 \right]^2 \left( \frac{n_p^l}{(n_p^2 + 1)^{l+2}} = p_0^{-3} \left( \frac{1 - \cos \alpha}{1 + \cos \alpha} \right)^l \left( \frac{1 + \cos \alpha}{2} \right)^{l+2} = p_0^{-3} \sin^l \alpha. \right.
\]  

(4.13)

Using this result in Eq.(4.10a), accounting for Eq.(4.10b) and the comparing the result with Eq.(4.6) we obtain:

\[
Y_{nlm}(\alpha, \theta, \phi) = 2^{l+1} \left[ \frac{\sin^l \alpha}{2\pi (n + l)!} \right] C_{n-l-1}^{l+1} (\cos \alpha) Y_{lm}(\theta, \phi).
\]  

(4.6b)

Obtained result is in perfect agreement with Eq.(4.6a), as promised.

These results allow us now to move further. In particular, we would like to consider a solution of the Schrödinger Eq.(3.19a) with potential Eq.(3.19b). D-O formally obtained its solution already in their first work, [7], for any \( \gamma \). We found, however, more convenient to discuss the same equation and its solution following [50]. In Eq.s(3.19a),(3.19b) and in [7],[50] this equation was treated as 3-dimensional while in [17] Ostrovsky did consider the 4 dimensional version of the same equation, but the obtained solution is not consistent with mathematically rigorous results of [89]. Therefore his results are to be reconsidered below.

4.4.2. Establishing an isomorphism between the Schrödinger equations with the fish-eye and the Coulomb potentials

4.4.2.1. A gentle introduction

In section 1 we noticed that initially Demkov and Ostrovsky [7] believed that ”Maxwell’s fish-eye problem is **closely related to** the Coulomb problem”. In section 3.5.2. we discussed the geometrical meaning of the stationary Schrödinger’s equation for the hydrogen atom.

Now it is time to reproduce Eq.(4.6a) with help of Eq.s(3.19a),(3.19b) \( \gamma = 1 \). By doing so we are going to replace the statement of D-O about ”close relationship” by the statement
“isomorphic”. Following [50], we reproduce Eq.s (3a), (3b) and (6) from this reference. Thus, we have

\[ \Psi(\rho, \theta, \varphi) = \text{const} \frac{\rho^{l+1}}{(1 + \rho^2)^{\frac{l+1}{2}}} C_{n-l-1}^{l+1}(\xi(\rho)) Y_{lm}(\theta, \varphi), \]

(4.14)

where \( \xi(\rho) = \frac{1 - \rho^2}{1 + \rho^2} \). A comparison between Eq.s (4.6a) and (4.14) suggests that we have to rewrite the factors containing the variable \( \rho \) accordingly. Fortunately, this can be done almost immediately by analogy with results displayed in Eq.s (4.11)-(4.14). Now we have to write \((np)^2 = \rho^2\), so that we obtain:

\[ \cos \alpha = \frac{1 - \rho^2}{1 + \rho^2}; \rho^2 = \frac{1 - \cos \alpha}{1 + \cos \alpha}; \rho^2 + 1 = \frac{2}{1 + \cos \alpha}. \]

(4.15a)

With help of these results we establish that \( \xi(\rho) = \cos \alpha \),

\[ \left( \frac{1 + \cos \alpha}{2} \right)^{\frac{2l+1}{2}} \left( \frac{1 - \cos \alpha}{1 + \cos \alpha} \right)^{\frac{l+1}{2}} = 2^{\frac{l+1}{2}} \sin^{l} \alpha \]

(4.15b)

Using these results in Eq.(4.14) brings us back to Eq.(4.6a) so that needed isomorphism is established, provided that we resolve the apparent paradox. Eq.s (3.19a), (3.19b) as well as Eq.s (3a), (3b) and (6) of [50] are manifestly 3 dimensional while the result, Eq.(4.6a), is 4 dimensional. It is also rather weird to have the 3-dimensional spherical harmonics \( Y_{lm}(\theta, \varphi) \) in the 4-dimensional result, Eq.(4.6). These circumstances prompt us to dig deeper into the issues just mentioned.

4.4.2.2. A peculiar relationship between 3 and 4 dimensional results

In the entire section 3 we dealt exclusively with the 3 dimensional versions of Eq.s (3.19a), (3.19b). In the already cited references, e.g., [7], [50], the 3 dimensional versions of Eq.s (3.19a), (3.19b) were treated and solved. Just above we noticed that these solutions carry information about the 4th dimension. It was left unnoticed in [7], [50] while in [17] Ostrovsky made an attempt to solve the 3-dimensional Eq.s (3.19a), (3.19b) by using the 3-sphere living in 4 dimensional Euclidean space (without justification for this step whatsoever). His results are not mathematically rigorous though. Below, we provide a detailed explanation. Notice that our demonstration has almost nothing in common with the celebrated 4-dimensional solution of the Schödinger equation for the hydrogen atom developed by Fock [92]. Nevertheless, the end result of our calculation will reproduce the 4-dimensional Eq.(4.6a) taken from [89]. Thus, we are about to uncover the "invisible" influence of the 4th dimension on solutions of 3-dimensional equations (3.19a), (3.19b). Our arguments are complementary to those by Fock [89].

We begin with the description of pentaspherical coordinates introduced in section 7 of our work [3]. This time, however, we shall provide additional details following [70] and [124], [134]. The pentaspherical coordinates had been discussed in accessible form in the monograph by
Felix Klein cited in [3]. Mathematical usefulness of these coordinates was recognized already by Böcher at the end of 19th century and was rediscovered at the end of the 20th century and further developed by Miller and collaborators [70]. Physical usefulness of pentaspherical coordinates was explained in [3]. For uninterrupted reading, we provide here some excerpts from [3] on this topic.

We begin with consideration of a sphere \( S^2 \) in \( \mathbb{R}^3 \). Analytically, the \( S^2 \) is described as
\[
x^2 + y^2 + z^2 - 2ax - 2by - 2cz + D = 0.
\]
(4.16a)
The radius \( r \) of the sphere is defined via
\[
r^2 = a^2 + b^2 + c^2 - D.
\]
(4.16b)
The introduced parameters are considered as coordinates in the space of spheres. In addition, it is convenient to introduce the homogenous (projective) coordinates
\[
a = \frac{\xi}{\nu}, b = \frac{\eta}{\nu}, c = \frac{\zeta}{\nu}, r = \frac{\lambda}{\nu}, D = \frac{\mu}{\nu}.
\]
(4.17)
These projective coordinates allow us to embed \( S^2 \) into projective space \( \mathbb{RP}^5 \) resulting in the equation
\[
\xi^2 + \pi^2 + \zeta^2 - \lambda^2 - \nu\mu = 0
\]
or, with \( \nu\mu = \alpha^2 - \beta^2 \), its analog
\[
\xi^2 + \pi^2 + \zeta^2 + \beta^2 - \lambda^2 - \alpha^2 = 0.
\]
(4.18a)
(4.18b)
Although in pentaspherical coordinates \( (x_1, ..., x_5) \) one uses a collection of 5 orthogonally intersecting spheres, just described mathematics remains very much the same. Specifically, the quadric, Eq. (4.18), now is written as the cone equation
\[
\sum_{i=1}^{5} x_i^2 = 0.
\]
(4.19)
Let \( (x, y, z) \in \mathbb{R}^3 \). Via stereographic projection (e.g. see Eqs (2.2),(2.3)) these Euclidean coordinates are related to the spherical coordinates \( (s_1, ..., s_4) \in S^3 \), \( \sum_{i=1}^{4} s_i^2 = 1 \). As in Eqs (2.2) and (2.3), we obtain analogously:
\[
x = \frac{s_1}{1 + s_4}, y = \frac{s_2}{1 + s_4}, z = \frac{s_3}{1 + s_4}
\]
(4.20a)
so that
\[
s_1 = \frac{2x}{r^2 + 1}, s_2 = \frac{2y}{r^2 + 1}, s_3 = \frac{2z}{r^2 + 1}, s_4 = \frac{1 - r^2}{1 + r^2}, r^2 = x^2 + y^2 + z^2.
\]
(4.20b)
Next, it is convenient to introduce the analog of Eq.s(4.17) by taking into account Eq.(4.19). Thus, we write:

\[ x_1 = 2X T, \ x_2 = 2Y T, \ x_3 = 2Z T, \ x_4 = X^2 + Y^2 + Z^2 - T^2, \ x_5 = i(X^2 + Y^2 + Z^2 - T^2). \] (4.21)

Accordingly,

\[ x = \frac{X}{T} = \frac{-x_1}{x_4 + i x_5}, \ y = \frac{Y}{T} = \frac{-x_2}{x_4 + i x_5}, \ z = \frac{Z}{T} = \frac{-x_3}{x_4 + i x_5}, \]

\[ x^2 + y^2 + z^2 - 1 = \frac{-2x_4}{x_4 + i x_5}, \ x^2 + y^2 + z^2 + 1 = \frac{2ix_5}{x_4 + i x_5}. \] (4.22)

Eq.s(4.21) imply (via duality) the following chain of equalities (taken from [93], page 403):

\[ \partial_X = 2T \partial_{x_1} + 2X \partial_{x_4} + 2iX \partial_{x_5}, \partial_Y = 2T \partial_{x_2} + 2Y \partial_{x_4} + 2iY \partial_{x_5}, \partial_Z = 2T \partial_{x_3} + 2Z \partial_{x_4} + 2iZ \partial_{x_5}. \]

Also,

\[ \partial_x = T \partial_X, \partial_y = T \partial_Y, \partial_z = T \partial_Z \] (4.24)

and, following [70], [93], we obtain as well:

\[ \partial_x = -(x_4 + i x_5) \partial_{x_1} + x_1(\partial_{x_4} + i \partial_{x_5}), \partial_y = -(x_4 + i x_5) \partial_{x_2} + x_2(\partial_{x_4} + i \partial_{x_5}), \]

\[ \partial_z = -(x_4 + i x_5) \partial_{x_3} + x_3(\partial_{x_4} + i \partial_{x_5}). \] (4.25a)

By replacing the quantum \(-i\partial_x\) by the classical \(p_x\), etc. we obtain the classical analog of Eq.(4.25a)

\[ p_x = -(x_4 + i x_5) p_{x_1} + x_1(p_{x_4} + ip_{x_5}), \]

\[ p_y = -(x_4 + i x_5) p_{x_2} + x_2(p_{x_4} + ip_{x_5}), \]

\[ p_z = -(x_4 + i x_5) p_{x_3} + x_3(p_{x_4} + ip_{x_5}) \] (4.25b)

The conformally flat space classical Hamiltonian \(H\) now reads

\[ H = p_x^2 + p_y^2 + p_z^2 + V(x) = 0 = (x_4 + i x_5)^2 \{ p_{x_1}^2 + p_{x_2}^2 + p_{x_3}^2 + p_{x_4}^2 + p_{x_5}^2 + V(x) \} = 0 \] (4.26a)

so that \((x_4 + i x_5)^2 \tilde{V}(x) = V(x)\). Now we adopt the quadric, Eq.(4.19), to \(S^3\). This is done by requiring \(x_5 = -i\). Accordingly, using Eq.(4.19) we obtain now

\[ \sum_{i=1}^{4} \frac{x_i^2}{-x_5^2} = 1, \]

implying \(s_1 = x_1\), etc. In view of this, Eq.(4.26a) can be rewritten as

\[ (x_4 + 1)^2 \{ p_{x_1}^2 + p_{x_2}^2 + p_{x_3}^2 + p_{x_4}^2 + V(x) \} = 0. \] (4.26b)
By comparing Eq.s (4.26a), (4.26b) with Eq.s (3.19a), (3.19b) adapted to the case \( \gamma = 1 \), we have to rewrite the potential, Eq.(3.19b) taking also into account Eq.(2.14b) and discussion which follow after this equation. Thus, we obtain:

\[
V(x) = \frac{(Ze^2)^2}{|E_n|} \left( \frac{1}{1 + r^2} \right)^2 |s_3 = (x_4 + 1)^2 \frac{(Ze^2)^2}{4|E_n|} \tag{4.27}
\]

In Eq.(4.26b) the combination \( p_{x_1}^2 + p_{x_2}^2 + p_{x_3}^2 + p_{x_4}^2 \) must be multiplied by the factor \( 1/2 \) in accord with the discussion following Eq.(2.14b). Furthermore, this combination represents not the flat Laplacian. This fact is fundamentally nontrivial. Its origin is based on the following chain of arguments. Using Eq.(4.26a) we have to require that \( p_{x_i} \) and \( x_i \) to be the canonically conjugate pair of variables. If, indeed, this is so then, say, at the classical level of description we have to calculate the Poisson bracket (P.B). Thus, we obtain:

\[
\{ \sum_{i=1}^{5} x_i^2, \mathcal{H} \}_P.B. = 2 (x_4 + ix_5)^2 \sum_{i=1}^{5} x_i p_i = 0. \tag{4.28}
\]

Adopted to \( S^3 \), Eq.(4.28) reads:

\[
\sum_{i=1}^{4} x_i p_i = 0. \tag{4.29}
\]

Thus, we have to solve Eq.(4.26b) subject to the constraint, Eq.(4.29). The solution of this problem is nontrivial. It is presented in the Appendix E. With help of obtained results, in the next subsection we shall recover the 4-dimensional hydrogen wave function, Eq.(4.6a).

### 4.4.2.3. Recovery of the 4-dimensional wave function, Eq.(4.6a), for the hydrogen atom

The 4-dimensional wave function, Eq.(4.6a), is presented in [86],[89]. In both references it was given without derivation. Therefore, we would like to restore needed details being guided by the results of our Appendix E, Ref.[94], and known quantum mechanical results for the 3-dimensional rigid rotator. At this point we need to extend these 3 dimensional results to the 4th dimensions. In 3 dimensions the well known Casimir operator \( \hat{L}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \) is used together with \( \hat{J}_z \) to label the spherical wavefunctions \( Y_{lm}(\theta, \phi) \). The first task now lies in finding the 4-d Casimir operator (or operators) analog(s) of \( \hat{L}^2 \). Fortunately, the results are presented in [89], pages 112-113. These are taken from [94],page 248. In Appendix E we argue that the 4-dimensional analogs of \( \hat{J}_x, \hat{J}_y \) and \( \hat{J}_z \) are the quantized Plücker coordinates, e.g. \( \hat{l}_{12}, \hat{l}_{13}, \hat{l}_{14}, \hat{l}_{23}, \hat{l}_{24} \) and \( \hat{l}_{34} \) so that \( \hat{L}^2 \) is replaced now by \( \hat{L}^2 = \hat{l}_{12}^2 + \hat{l}_{13}^2 + \hat{l}_{14}^2 + \hat{l}_{23}^2 + \hat{l}_{24}^2 + \hat{l}_{34}^2 \). Explicitly, in terms of the spherical coordinates defined in Eq.(4.7) we obtain:

\[
\hat{L}^2 = -\frac{\partial^2}{\partial \alpha^2} - 2 \cot \alpha \frac{\partial}{\partial \alpha} - \frac{1}{\sin^2 \alpha} \left[ \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right]. \tag{4.30a}
\]
Notice, however, that 

\[ \hat{L}^2 \hat{Y}_{lm}(\theta, \varphi) = \hbar^2 l(l + 1) Y_{lm}(\theta, \varphi). \]

Because of the known relation

\[ \hat{L}^2 = -\frac{\hbar^2}{2} \sin^2 \theta \frac{\partial^2}{\partial \theta^2} \cos \theta - \cot \theta \frac{\partial}{\partial \theta} + \frac{\hbar^2}{2} \sin^2 \varphi \frac{\partial^2}{\partial \varphi^2}, \]

Eq.(4.30a) should be rewritten accordingly as

\[ \hat{L}^2 = -\frac{\partial^2}{\partial \alpha^2} - 2 \cot \alpha \frac{\partial}{\partial \alpha} + \frac{1}{\sin^2 \alpha} \hat{L}^2, \quad (4.30b) \]

By analogy with 3 dimensions, in 4 dimensions we write instead:

\[ \hat{L}^2 Y_{nlm}(\alpha, \theta, \varphi) = I_{nl} Y_{nlm}(\alpha, \theta, \varphi). \quad (4.31a) \]

The eigenvalue \( I_{nl} \) is to be determined from the equation

\[ \frac{l(l + 1)}{\sin^2 \alpha} - \frac{\partial^2}{\partial \alpha^2} - 2 \cot \alpha \frac{\partial}{\partial \alpha} \Psi_{nl}(\alpha) = I_{nl} \Psi_{nl}(\alpha). \quad (4.32) \]

in which, in view of Eqs.(4.30b),(4.31a), we have to present \( Y_{nlm}(\alpha, \theta, \varphi) \) as \( \Psi_{nl}(\alpha) Y_{lm}(\theta, \varphi) \).

Since the obtained equation is equivalent to Eq.(4.26b), we should make an identification:

\[ I_{nl} = -\frac{(\text{Ze})^2}{2|E_n|}. \]

Next, we let \( x = \cos \alpha \) in Eq.(4.32). Then, we write \( \Psi_{nl}(\alpha) = (1 - x^2)^{\frac{l}{2}} F_{nl}(\alpha) \). With help of these substitutions Eq.(4.32) acquires the following look

\[ (1 - x^2) \frac{d^2}{dx^2} F_{nl} - (2l + 3)x \frac{d}{dx} F_{nl} + [I_{nl} - l(l + 2)] F_{nl} = 0. \quad (4.33) \]

This equation should be compared against the canonical equation for the Gegenbauer polynomials [95]:

\[ (1 - x^2) \frac{d^2}{dx^2} C_n^{(\lambda)}(x) - (2\lambda + 1)x \frac{d}{dx} C_n^{(\lambda)}(x) + n(n + 2\lambda)C_n^{(\lambda)}(x) = 0. \quad (4.34) \]

Upon comparison between these two equations, we obtain: \( (2l + 3) \equiv (2\lambda + 1) \) implying \( \lambda = l + 1 \). Also, \( n(n + 2\lambda) \equiv I_{nl} - l(l + 2) \) implying \( I_{nl} = (n + l + 1)^2 - 1 \). Let now \( n + l + 1 = 2F + 1 \) then, \( (n + l + 1)^2 - 1 = 4F(F + 1) \). This result should be compared with those presented in [86], [89]. For this it is sufficient to relabel \( n + l + 1 \) as \( \hat{n} \). By comparing with standard physics literature on hydrogen atom, we have to relabel \( n \) as \( n_r \), where \( n_r \) is the radial quantum number. Such an identification between \( n \) as \( n_r \) is plausible but misleading even though it is present in all works by D-O and those who used the D-O works. Explanation is given at the end of section 5.
With such a background, we obtain: \( \hat{n}^2 - 1 = 4F(F+1) \). On page 5 of [89] we find that the 4 dimensional wave functions \( \hat{Y}_{nlm} \) (e.g. see Eq.(4.31)) are belonging to the eigenvalue \( \hat{n}^2 - 1 \) as required. Next, we obtain: \( n_r = 2F - l \) implying \( F \hat{n}l(\alpha) = \frac{c_l}{2}F^{-l}(\cos \alpha) \). Since \( \Psi_{nl}(\alpha) = (1-x^2)^{\frac{l}{2}} F_{nl}(\alpha) \), we obtain as well \( \Psi_{nl}(\alpha) = const(\sin \alpha)C_{l+1}^{2F-l}(\cos \alpha) \). Finally, since \( Y_{nlm}(\alpha, \theta, \varphi) = \Psi_{nl}(\alpha)Y_{lm}(\theta, \varphi) \), we end up (accounting for the normalization, Eq.(4.8)) with the wave function, Eq.(4.6a), as required.

4.4.2.4. Schrödinger-assisted recovery of the eigenvalue spectrum for hydrogen atom

Calculation of the eigenvalue spectrum for hydrogen atom can be found in any textbook on quantum mechanics. Here, we approach this problem nontraditionally. In doing so, we borrow some ideas from the obscure paper by Schrödinger [96] (circa 1940) superimposed with results of our Appendix F. Schrödinger was interested in finding the extent to which the effects of curvature of Universe may affect the spectrum of hydrogen atom. Schrödinger choose to consider the Keplerian motion on the hypersphere \( S^3 \) of radius \( R \). Fundamentally interesting for us is to read about the rationale of his calculation. In his paper we find the following passages:

"It may appear foolish to pay attention to the extremely feeble curvature of the Universe in dealing with the hydrogen atom, because even the influence of those much stronger fields of gravitation in which all our observations are actually made (if the frame is properly chosen) entirely negligible. But this problem, by obliterating the sharp cut between ” elliptic and hyperbolic orbits”(the classical orbits are all closed) and by resolving the continuum spectrum into intensely crowded line spectrum, has extremely interesting features, well worth investigating..."

By looking for spaces in which all classical orbits are closed, Schrödinger actually was looking at

a) Bläshke manifolds discussed in Appendices A and B,

b) Superintegrable dynamical systems discussed in this and next sections,

c) Bertrand spaces to be discussed in the next section.

He begins his calculations with the equation on \( S^3 \) (not on \( R^3! \))

\[
\frac{\hbar^2}{2mR^2}
\left[
-\frac{1}{\sin^2 \alpha} \frac{d}{d\alpha} (\sin^2 \alpha \frac{dS}{d\alpha}) + \frac{l(l+1)}{\sin^2 \alpha} S
\right]
\frac{e^2}{R} S \cot \alpha - ES = 0.
\]

A quick look at our Eq.(4.30b) allows us to rewrite Eq.(4.35a) into more familiar form as follows

\[
\frac{\hbar^2}{2mR^2} \hat{L}^2 S = ES + \left[\frac{e^2}{R} \cot \frac{\alpha}{2}\right] S.
\]

In this equation we corrected Scrodinger’s result: in going from \( R^3 \) to \( S^3 \) of radius \( R \) he replaced the Coulombic 3-dimensional term \( \frac{e^2}{R} \) by \( \frac{e^2}{R} \cot \alpha \). The correct result is: \( \frac{e^2}{R} \cot \frac{\alpha}{2} \).

It is worthy of demonstrating how this result is actually obtained. Using Eq.(4.20b) we write:

\[
r^2 = \frac{1 - s_4}{1 + s_4}.
\]
Hence,

\[
\frac{1}{r} = \left( \sqrt{\frac{1 - s_4}{1 + s_4}} \right)^{-1} = \sqrt{\frac{(1 + s_4)^2}{1 - s_4^2}}
\]  

(4.37a)

Taking into account that \( s_4 = x_4 = R \cos \alpha \). Let \( R = 1 \), then we obtain:

\[
\frac{1}{r} = \frac{1 + \cos \alpha}{\sin \alpha} = \frac{2 \cos^2 \frac{\alpha}{2}}{2 \sin \frac{\alpha}{2} \cos \frac{\alpha}{2}} = \cot \frac{\alpha}{2}.
\]  

(4.37b)

In our calculations we want to take advantage of the Coulomb-fish-eye isomorphism. Therefore, being guided by this isomorphism, instead of the factor \( e^2 R \cot \frac{\alpha}{2} \) we systematically used the factor \( -\frac{(Ze^2)^2}{2|E_n|} \). This caused us to obtain the eigenvalue spectrum \( I_{nl} \) correctly in agreement with [86], [89]. However, this is not yet the spectrum for hydrogen atom. To obtain this spectrum we use the results of Appendix F. These are also allowing us to make a connection between our current results and those by Schrödinger. This is achieved with the amended Eq.(4.31a), that is, in view of Eq.(4.35b), with

\[
\hat{L}^2 Y = (I_{nl} - E)Y
\]  

(4.31b)

The choice of \( E \) is determined by replacing \( I_{nl} = \hat{n}^2 - 1 = 4F(F + 1) \) by \( I_{nl} - E = 4F(F + 1) \). From Appendix F we know that the parameter \( E \) can be chosen once and for all based on physical considerations. In our case, it is sufficient to chose \( -E = -1 \). With this choice we obtain:

\[
-\frac{(Ze^2)^2}{2|E_n|} = (2F + 1)^2 \text{ or } E_n = -\frac{(Ze^2)^2}{2(2F + 1)^2}, F = 0, \frac{1}{2}, 1, ...
\]  

(4.38)

This result coincides with that given on p.645 of [86] as required.

Remark 4.8. In the limit \( R \to \infty \) the spectrum obtained by Schrödinger correctly reproduces the spectrum of hydrogen atom. However, the calculated wavefunctions differ from the standard, Eq.(4.6a). Since in this section we obtained both the eigenfunctions and eigenvalues for hydrogen atom correctly using methods and arguments different from those used by Fock [92], we leave for our readers to investigate further two topics. a) What made Schrödinger to use 4-dimensional calculations instead of 3-dimensional? Unlike Fock, who clearly stated the reason for using 4 dimensional calculations for hydrogen atom, Schrödinger, being apparently not aware of Fock’s results, bypassed this issue altogether. b) It is of interest to recover the wavefunctions for hydrogen atom, Eq.(4.6a), using Eq.(4.35a).

4.5. The role of Hopf mapping in emerging picture

4.5.1. What is the Hopf mapping and why it is essential for development of our formalism

\[\text{Bertrand curved spaces of section 5 are 3 dimensional.}\]
The entire section 3 and a large part of Appendix F is devoted to the issues related to conformal invariance. Previously we mentioned the work by Makowski [54]. He took advantage of the fact that in 2 dimensions the Laplacian is conformally invariant. This fact enabled him to solve the 2-dimensional Sturmian Eq.(3.1b) for the fish-eye-type potentials exactly. In 3 dimensions the Laplacian no longer possess the property of conformal invariance. To bypass this difficulty the conformally invariant (Yamabe) Laplacian should be used instead. This fact created a lot of technical difficulties but allowed us to demonstrate in detail the full power of Hadamard-style calculations. These were only outlined in [3]. Such calculations are of significance not only for our work. To our knowledge, they have not been exposed in sufficient detail in physics literature, perhaps with exception of gravitation. But even in this field the alternative route of bypassing the issue of conformal invariance in 3 dimensions was not discussed also. It is associated with the systematic uses of the Hopf mapping. This mapping is not a novel item in physics literature [97]. Nevertheless, to our knowledge, the aspects we are willing to discuss are new. Because of this, they will be studied further in detail in Part II.

The idea of Hopf mapping is simple. Take the equation for the 3 sphere, \( S^3 \) living in \( \mathbb{C}^2 \), e.g. \( |z_1|^2 + |z_2|^2 = 1 \), \( z_i = x_i + iy_i \), \( i = 1, 2 \), and look for the ratio \( Z = \frac{z_1}{z_2} \) (or \( Z = \frac{z_2}{z_1} \)). While \( S^3 \in \mathbb{C}^2, Z \in \mathbb{C} \). But \( \mathbb{C} \cup \infty = S^2 \)! From here follows the Hopf map: \( S^3 \to S^2 \). Subsequently the map \( S^2 \to S^3 \) was also designed and used, e.g. read [98], etc. In the previous subsection using the pentasperical coordinates we mapped the 3 dimensional Sturmian problem involving Eq.(3.19) into \( S^3 \). We want now to reanalyze the 2 dimensional results by Makowski [54] using the notion of Hopf map. It should be noticed, though, that Makowski used the 2 dimensional plane in his work. With help of conformal invariance his results can be lifted to \( S^2 \). E.g. look again at Eq.s(2.15)-(2.22) and (3.1a,b). The first thing we have to check: will his results reproduce known 2 dimensional results for the hydrogen atom. The answer depends upon our ability to solve the following problem.

4.5.2. Solution of the Sturmian problem for hydrogen atom on \( S^2 \)

On \( S^2 \) the potential, Eq.(3.19b), is constant. In fact, it is the same constant as in previous subsection: \( \tilde{V}(x) = -\frac{(Ze^2)^2}{2|E_n|} \). The Laplacian restricted to \( S^2 \) is describing the rigid rotator. Therefore, we again run into the familiar equation: \( \hat{L}^2 Y_{lm}(\theta, \varphi) = \hbar^2 l(l+1)Y_{lm}(\theta, \varphi) \). The question remains: will this equation reproduce the 2-d hydrogen spectrum? Very fortunately, positive answer was found in [99]. These authors had adapted Pauli’s dynamical group-theoretic method for solving hydrogen atom to the case of 2 dimensions. By repeating the same steps, they indeed arrived at the rigid rotator equation. The Pauli-like group algebra enabled them to arrive at the equation for the spectrum

\[
l(l + 1) = \left(-\frac{1}{4} + \frac{1}{E}\right)
\]  

(4.39a)
leading to the known result:

$$E_l = -\frac{1}{(l + \frac{1}{2})^2}, \ l = 0, 1, 2, ...$$  \hspace{1cm} (4.39b)

For the future reference, the 3-dimensional result taken from [86] and used in Eq.(4.38) is given as follows:

$$F(F + 1) = -(\frac{1}{4} + \frac{1}{8E}), \ F = 0, 1/2, 1, ...$$  \hspace{1cm} (4.40)

leading to

$$E_F = -\frac{1}{2n^2}; \ n = 2F + 1 = 1, 2, 3, ...$$

Both results can be made identical if one notices that Eq.(4.39a) uses only the angular momentum interpretation of the standard commutator algebra \( [\hat{J}_j, \hat{J}_k] = i\varepsilon_{jkl}\hat{J}_l \). In the case if the same commutator algebra is interpreted spin-theoretically, the results Eq.(4.39b), (4.40) will coincide. This is becoming permissible in the case if the 2-dimensional results for \( S^2 \) are lifted to \( S^3 \) using the inverse Hopf map. We expect that the rest of 2-dimensional results will follow the same trend.

4.5.3. Closer look at the rigid rotator equation

4.5.3.1. Calculation of eigenfunctions

The purpose of this subsection is to demonstrate close relation between results of subsection 4.4.2.3. and those which follow from the equation for 3-dimensional rigid rotator. Such an equation is well known in quantum mechanics under the name of equation for the associated Legendre polynomials \( P^m_l(x) \). In terms of the variable \( x = \cos\theta \) the equation for these polynomials reads:

$$\left(1 - x^2\right)\frac{d^2}{dx^2}P^m_l(x) - 2x\frac{d}{dx}P^m_l(x) + \left[l(l + 1) - \frac{m^2}{1 - x^2}\right]P^m_l(x) = 0.$$  \hspace{1cm} (4.41)

It should be compared with Eq.(4.32). By analogy with Eq.(4.32) we shall look for a solution of Eq.(4.41) in the form \( P^m_l(x) = (1 - x^2)^{\frac{m}{2}}\tilde{P}^m_l(x) \). Substitution of this ansatz into Eq.(4.41) leads to [100]

$$\left(1 - x^2\right)\frac{d^2}{dx^2}\tilde{P}^m_l(x) - 2(m + 1)x\frac{d}{dx}\tilde{P}^m_l(x) + [l(l + 1) - m(m + 1)]\tilde{P}^m_l(x) = 0.$$  \hspace{1cm} (4.42)

But this is an equation for the Gegenbauer polynomials, Eq.(4.34)! In the simplest case, \( m = 0 \), we obtain: \( P^0_l(x) = C^l_n(x), n = l \). For \( m \neq 0 \), we have to put \( \lambda = m + 1/2 \) in Eq.(4.34) and \( l - m = n \) in Eq.(4.42) (to be compared with Eq.(4.34)) implying \( \tilde{P}^m_l(x) = C^{m+\frac{1}{2}}_n(x) = C^{m+\frac{1}{2}}_{l-m}(x) \). These results we would like to compare against Eq.(9) of Makowski [54]. To do so, it is sufficient to make an identifications : Makowski’s \( \lambda \mapsto m \), also his \( n_r + \lambda \mapsto n + m \). We are warning our readers not to confuse the factor \( \lambda \) in Gegenbauer’s
Eq.(4.34) and the factor $\lambda$ in Makowski’s paper [54]. Evidently, our $n$ is the same as his $n_r$. Up to a complex factor $\exp(\pm im\varphi)$ the solution obtained by Makowski is given by

$$\psi_{n_r}(x,y) = \text{const}(1 - \xi^2)^{\frac{\lambda+\frac{1}{2}}{2}}C_{n_r}^{\lambda+\frac{1}{2}}(\xi), \quad \xi = \frac{1-r^2}{1+r^2} = \frac{1-z^2}{1+z^2}. \quad (4.43a)$$

Here we used our Eq.s (2.15)-(2.22) to write his Eq.(9) in our notations. This allows us to take into consideration that $\xi = \frac{1-r^2}{1+r^2} = Z = \cos \theta$ resulting in

$$\psi_{n_r}(\theta, \varphi) = N'(\sin \theta)^m C_{n_r}^{m+\frac{1}{2}}(\cos \theta). \quad (4.43b)$$

Using Eq.(2.15), it is clear, that $x = \cos \theta \rightleftharpoons Z$. In addition, $N$ is the normalization constant. We would like to compare Makowski’s 2 dimensional result, Eq.(4.39a) (or Eq.(4.39b)), against that coming from the equation for the rigid rotator, Eq.(4.42). This equation is leading us to the solution

$$\psi_n(\theta, \varphi) = N'(\sin \theta)^m C_{l-m}^{m+\frac{1}{2}}(\cos \theta). \quad (4.44)$$

Since we just defined $l-m = n$ and $n = n_r$, this identification causes us to write $N' = N$. Makowski’s result, Eq.(4.43b) was obtained using planar geometry while the result, Eq. (4.44), was obtained using the geometry/topology of $S^2$. Use of stereographic projection connects these two geometries. When it comes to the connection between the respective differential equations - on $\mathbb{C}$ and on $S^2$ - use of conformal invariance in Eq.(3.1b) is essential since the stereographic projection is a conformal mapping. Should the potential in the planar Schrödinger equation be zero, the mapping $\mathbb{C} \rightleftharpoons S^2$ would transform the flat Laplacian to the Laplacian on $S^2$. The Sturmian problem on $\mathbb{C}$ is the eigenvalue problem for the Laplacian on $S^2$. It is the familiar eigenvalue problem for the rigid rotator in quantum mechanics.

It is always possible to adapt the 3-dimensional Eq.(3.19) to $S^2$ as long as the conformal transformations are not involved. When they are involved, we only can lift Eq.(3.1b) to $S^2$ but we cannot make a reduction from 3 dimensions to 2 since in 3 and higher dimensions we are dealing with the conformal (Yamabe) Laplacian while in dimension 2 - with the ordinary Laplacian which is conformally invariant (only in 2 dimensions). But we can use the stereographic projection from: from $S^3$ to $\mathbb{R}^3$. Because of this, it is of interest to compare conformally modified planar results by Makowski and Pepowski [49] against the analogous 3-dimensional (actually the 4-dimensional, as demonstrated in previous subsection) results of Ref.[50]. Such a comparison will give us an idea about the extent to which results on $S^2$ by Makowski [54], actually done on $\mathbb{C}$, change when they are lifted (via the Hopf map) to $S^3$.

It should be noted though that we have not constructed yet the Hopf map. This is done in mathematical literature already and will be adapted for our needs in Part II.

4.5.3.2. Calculation of the spectrum
To complete our calculation we need to reproduce Eq.s(4.39b). We shall proceed analogously to the methodology developed in subsection 4.4.2.4. For this purpose we have to replace now the equation
\[
\frac{L^2}{\hbar^2} Y_{lm}(\theta, \varphi) = I_{lm} Y_{lm}(\theta, \varphi)
\] (4.45a)
by
\[
\frac{L^2}{\hbar^2} Y_{lm}(\theta, \varphi) = (I_{lm} - E) Y_{lm}(\theta, \varphi)
\] (4.45b)
where we have to choose, as before, \(I_{lm} = -\frac{(Ze^2)^2}{2|E_n|}\) and select \(E = -\frac{1}{4}\). This choice follows from the identification
\[
l(l + 1) = -\frac{(Ze^2)^2}{2|E_n|} - \frac{1}{4}
\] (4.46a)
done with help of accounting for Eq.(4.42) and the property \(l(l + 1) + \frac{1}{4} = (l + \frac{1}{2})^2\). Using these results we finally arrive at the equation for spectrum
\[
E_l = -\frac{(Ze^2)^2}{(l + \frac{1}{2})^2}, l = 0, 1, 2, ...
\] (4.46b)
Obtained result is in accord with Eq.(4.39b) as required. Furthermore, in the system of units \(\hbar = 1, m = 1\), the obtained result exactly coincides with that reported in [101].

4.5.4. Comparison between the 2 dimensional results of Ref.[49] and 4 dimensional results of [50].

We begin with the discussion of conformally deformed 2-dimensional results presented in [49]. They are immediately linked with results by the same authors discussed in previous subsection. Instead of duly reproducing the results of [49], we approach the whole problem differently. That is, first, in the absence of potential we lift the flat Laplacian from \(C^2\) to \(S^2\). The conformal invariance is compatible with such a lift as we already know, e.g. see Eq.(3.1). Before performing any conformal transformation we notice that the potential \(\tilde{V}(x)\) must be replaced by \(l(l + 1)\) in Eq.(4.45) in accord with theory of 2 dimensional rigid rotator as discussed in previous subsection. To study the effects of conformal transformations we analyze Eq.(5) of [49] by the same methods as we used in Eq.s(4.11)-(4.15). In the present case we start with
\[
F_{nl}^{(k)}(\xi) = N_{nl}^{(k)} (1 - \xi^2)^{1/2} C_n^{l/\gamma + 1/2}(\xi), \xi = \frac{1 - r^{2\gamma}}{1 + r^{2\gamma}}.
\] (4.47a)
To be compatible with our notations we replaced the \(k\)- factor in [49] by the \(\gamma\) factor defined in our Eq.(3.19). Before performing any conformal transformation we put \(\gamma = 1\) in the above result to check it against Makowski’s Eq.(4.43b) (see above). By comparing Eq.s (4.43)
and (4.47a) we notice that \( l \) in Eq.(4.47a) must be replaced by \( m \). If we treat \( r^\gamma = \rho \) as independent variable, we still can use \( \xi = \cos \theta = x \). Accordingly, we obtain:

\[
F_{nm}^{(\gamma)}(\theta) = N_{nm}^{(\gamma)} (\sin \theta)^{m/\gamma} C_{n}^{m/\gamma+1/2}(\cos \theta), n = n_r.
\]  

(4.47b)

For \( \gamma = 1 \) Eqs.(4.43b) and (4.47b) coincide as required. Use of conformal transformations causes us to make a replacement \( m \rightarrow m/\gamma \) in Eq.(4.43b) to reach an agreement with Eq.(4.47a). Such a replacement makes perfect physical sense because in this work the azimuthal quantum number, the wave function boundary condition \( \Psi(0) = \Psi(2\pi) \) prior to conformal mapping must be preserved after the conformal mapping is performed. This requirement is the cause of the transformation: \( m \rightarrow m/\gamma \).

Now we are ready to analyze the 4-dimensional results of Ref. [50], page 34. For \( \gamma = 1 \) this was done already in Eqs (4.14),(4.15). Therefore, only the conformally deformed case is treated in this subsection. It is treated by analogy with that we just discussed when we considered the case of 2 dimensions. The additional help is coming from Eqs(4.14),(4.15). Thus, now we obtain:

\[
\cos \alpha = \frac{1 - \rho^{2\gamma}}{1 + \rho^{2\gamma}}; \rho^{2\gamma} = \frac{1 - \cos \alpha}{1 + \cos \alpha}; \rho^{2\gamma} + 1 = \frac{2}{1 + \cos \alpha};
\]

(4.48a)

\[
(1 + \cos \alpha)^{\frac{2l+1}{2}} (1 - \cos \alpha)^{\frac{l+1}{2}} = 2 \frac{2l+1}{2} \sin^2 \alpha
\]

(4.48b)

Eq.(4.14) is replaced now by

\[
\Psi(\alpha, \theta, \phi) = \text{const}' (\sin \frac{\theta^l}{\gamma} \alpha) C_{\frac{2l+1}{2}}^{\frac{1}{2}+\frac{1}{2}}(\cos \alpha) Y_{l m}(\theta, \phi).
\]  

(4.49a)

Here, in accord with authors of [17] and[50], \( M = n + (\gamma^{-1} - 1)l \). For \( \gamma = 1 \) Eq.(4.49a) coincides with Eqs.(4.14),(4.15) as required. Next, we compare this (4-dimensional) result against the 2-dimensional result, Eq.(4.47b), that is with

\[
F_{nm}^{(\frac{1}{2})}(\theta) = N_{nm}^{(\frac{1}{2})} (\sin^{2m} \theta) C_{n_r}^{2m+1/2}(\cos \theta).
\]  

(4.47c)

In such a form we compare it now against Eq.(4.49a) in which we should put \( \gamma = 1/2 \):

\[
\Psi(\alpha, \theta, \phi) = \text{const}' (\sin^{2l} \alpha) C_{n_r}^{2l+1/2} (\cos \alpha) Y_{l m}(\theta, \phi).
\]  

(4.49b)

This result is written in terms of notations used in [17] and [50]. In these references \( M = n + (\gamma^{-1} - 1)l \) and, we have to write now \( \gamma = 1/2 \), and to use the standard result: \( n = n_r + l + 1, n_r = 0, 1, 2, ... \) The comparison implies that for \( \gamma = 1/2 \) the 4 dimensional wave
function $\Psi(\alpha, \theta, \varphi)$ can be obtained with help of 2 dimensional $F_{n,m}^{(\frac{1}{2})}(\theta)$ if we take into account that 3-dimensional $z = \cos \theta$ is equal to $t = \cos \alpha$ in 4 dimensions, e.g. see Eq.(4.7). Therefore we should make a replacement $\theta \rightleftharpoons \alpha$ wherever this is appropriate. Next, we have to make a replacement $m \rightleftharpoons l$ and, finally, we have to use the addition formula [100], page 121,

$$C^\alpha_\alpha + \beta(x) = \sum_{m=0}^{n} C^\alpha_m(x)C^\beta_{n-m}(x).$$

(4.50)

After these replacements and use of the addition formula the final result should be multiplied by $Y_{lm}(\theta, \varphi)$. In the end, the obtained result must be properly normalized with help of the normalization condition for the Gegenbauer polynomials

$$\int_0^\pi d\alpha \left( \sin 2^p \alpha \right) \left[ C^p_l(\cos \alpha) \right]^2 = \frac{\pi \Gamma(2p + 1)}{2^{2p-1}l!(l+p)\Gamma^2(p)}.$$  

(4.51)

In writing the above results, following works by D-O and those who extended their works, we silently assumed that everything is fine with the result, Eq.(4.49a). But this is not at all the case. Mathematically correct results are presented in the following subsection

4.6. Calculation of the deformed spectrum in 4 dimensions. Emergence of the Madelung rule

4.6.1. General comments

Calculation of the deformed spectrum is technically easy but, for the results to make physical sense, prior discussion is absolutely essential. For readers convenience, needed background material is given in the Appendix G. In it we explain what is wrong with the existing "proofs" of the Madelung rule. We also describe the unexpected Hartree-Fock origins of the conformally deformed fish-eye potential, Eq.(3.19), with $\gamma = 1/2$. The description of this connection with Hartree-Fock contributions to the effective potential $V_{eff}(r)$, Eq.(1.3), cannot be found among D-O papers cited thus far. Nevertheless, D-O did mention this connection in [102] and [103] but only in the context of the Thomas-Fermi (T-F) theory. The Appendix G does contain an information about the connection with the Hartree-Fock results. Yes, it is true that the contributions to the T-F theory made by Tietz resulted in the potential, Eq.s(G.8), (G.9), bearing his name. It is also true that, up to a constant factor, analytically this potential is the same as the deformed fish-eye potential, Eq.(3.19) with $\gamma = 1/2$. But D-O have not cited results by other authors in which it is demonstrated that the combined use of the Coulombic and Hartree-Fock contributions to the effective potential $V_{eff}(r)$, Eq.(1.2), results in the deformed fish-eye potential with $\gamma = 1/2$.

The problem of solving Eq.(1.2) had began with the work by Slater. In his 1932 paper [104] he writes ”For any detailed calculations dealing with atomic or molecular structure, good approximations to the atomic wave functions are essential. The most satisfactory method, in general, for building up such functions to be by the use of one-electron functions
which are solutions of the problem of an electron moving in a central field...” A noticeable advancement in this direction was made by Latter in 1955 [26]. He numerically solved Eq.(1.2) using the Thomas-Fermi-Dirac type potential for all elements with \( Z = 1 \div 92 \). Latter noticed that” The important error in this application of a fixed central field potential arises just from the use of the same potential for all configurations of the atom. This error clearly grows with increasing excitation of the atom above the ground state....The statistical potentials give acceptable values for ground state energies and, presumably, will therefore give semiquantitative predictions for states of low excitation.” Results by Latter had been further analyzed by March. In his book [27] on p.76 March writes "In a Coulomb field we would, of course, fill the K, L, M shells successively. The closed shell of principal quantum number \( n \) holds \( 2n^2 \) electrons and hence shells close, for a Coulomb field, for 2,10, 28, etc. electrons .... Now, in real atoms, the closed shell configurations occur of He \((Z=2)\) and Ne \((Z=10)\) which fit the Coulomb field scheme. But the next rare gas is Ar, with 18 electrons....

a screened Coulomb field such as given by Hartree or a Thomas-Fermi theory leads for an atomic number \( Z=18 \) to the filling of 3p sub shell which is rather far from the 3d level. Also, for larger atomic number, level crossing occurs. The principal quantum number is no longer precise enough to group the energy levels: for a screened Coulomb field these depend upon \( n \) and the orbital angular momentum quantum number \( l \).” Thus, without using the word "Madelung rule", March recognized that the accurate calculations by Latter [26] provide the strongest possible justification of the validity of Madelung rule! It should be kept in mind that Latter compared Thomas-Fermi and Thomas-Fermi-Dirac solutions for energies of individual electrons against the available Hartree and Hartree-Fock results for respective atoms. All results by Latter are obtained numerically and are based on numerical solution of Eq.(1.2) with the Thomas-Fermi-Dirac type effective potential \( V_{eff}(r) \). They demonstrate a very remarkable agreement with the Hartree and Hartree-Fock results. The solutions were obtained numerically because Latter was not using the Tietz potential. As discussed in the Appendix G, the Tietz potential is of Thomas-Fermi type but is of convenient analytical form and fits very nicely the Hartree-Fock data for the effective potential [25], p.664,Fig.10. Contrary to D-O descriptions of the Tietz work, Tietz recognized the qualities of his potential immediately after he discovered it. This caused him to apply the methodology developed by Kerner [105] in 1951 to the potential Tietz discovered later on. At the same time, Kerner, after consulting with Bethe and Feynman, obtained the exact analytical solution for the stationary Schrödinger equation having the potential \( V_{eff}(r) = -\frac{Ze}{r} \sqrt{\varphi(x)} \). Here \( \varphi(x) \) is the same as in Eq.(G.8), except that Kerner was fiddling with the constant \( \alpha \) (to get the best possible agreement with experiment) while in Eq.(G.8) this constant is fixed by the logic of the T-F calculations. Kerner tested his effective potential against the numerically obtained Hartree potential and found astonishingly good agreement as demonstrated in [105], Fig.1, page 71. Subsequently, Titz adapted word-for-word Kerner’s methodology for solving the Schrödinger’s equation with the potential \( V_{eff}(r) = -\frac{Ze}{r} \varphi(\frac{r}{a}) \). In [29] the latest attempt by Tietz at solving this type of Schrödinger equation is presented along with the list of all his previous attempts at exact solution. Unlike Latter, Kerner had not calculated the spectrum
for all $Z$’s and for many $l$’s. He fixed his attention on the Mercury ($Z = 80$) and made a comparison of a single electron eigenvalues (for various $n$’s and $l$’s) calculated by his exact method against the relevant Hartree-type calculations. He obtained a good agreement with the Hartree results summarized in the Table II, page 74, of [105]. Kerner has no mention of the Madelung rule in his paper. Following into footsteps of Kerner, Tietz also selected Mercury for his study and compared his exact (Kerner-style) calculations against those published in Kerner’s paper. Naturally, a good agreement with experimental data was also obtained.

D-O entered into research on this topic only in 1971-1972. Unlike other authors, they recognized the importance of restrictions caused by the Bertrand theorem and they reinterpreted the Tietz potential, without mentioning Tietze’s name and his works, as the conformally deformed Maxwell’s fish-eye potential. This is explained in section 2. This caused them to restrict their treatment [7],[17],[25] aimed at the proof of Madelung rule to studies of the Schrödinger equation (with Tietz potential ) to the $E = 0$ case only. The rationale for doing so is discussed in sections 1−3 of our paper. Already in section 2 we explained that the Schrödinger equation with the fish-eye potential should be used with $E = 0$ by design. This requirement has nothing to do with the energy spectrum of hydrogen atom though. This was demonstrated in subsection 4.4.2.4. But it has everything to do with the conformal invariance of the underlying Eq.(3.19) allowing to conformally deform the Maxwell fish-eye potential thus allowing to study the multielectron atoms with help of the same formalism. Being unaware of just described facts, especially those, in Appendix F, D-O studied only the $E = 0$ solution of the Schrödinger equation with the Tietz potential. At the same time, following the methodology developed by Kerner, Tietz obtained the exact solution of the same equation as studied by D-O in his 1956 paper [28] without any restrictions on $E$. The D-O method of solution of Eq.(3.19) differs from that by Tietz and, therefore, by Kerner. The analytical form of the wave function, Eq.(4.49b), is absent in the paper by Tietz.

4.6.2. Derivation of the low lying spectrum of multielectron atom consistent with the Madelung rule

The above information along with results from Appendix G makes it possible to calculate the deformed spectrum at this point. We proceed by analogy with results obtained in subsections 4.4.2.4 and 4.5.3.2. To use these results, we should also consult the development in subsection 4.4.2.3. This brings us back to the deformed wave function Eq.(4.49b). The question emerges: Will this function be an eigenfunction of Eq.(4.31a)? A quick look at the analogous eigenfunction, Eq.(4.6a), and taking into account that $Y_{nlm}(\alpha, \theta, \varphi) = \Psi_{nl}(\alpha)Y_{lm}(\theta, \varphi)$, with $\Psi_{nl}(\alpha) = (1-x^2)^{\frac{l}{2}}F_{nl}(\alpha), x = \cos \alpha$ leads us to the following observation.

Use of the factor $(1-x^2)^{\frac{l}{2}} = \sin \alpha$ in $\Psi_{nl}(\alpha)$ and substitution of the ansatz $\Psi_{nl}(\alpha)Y_{lm}(\theta, \varphi)$ into Eq.(4.31a) allows us to get rid of the denominator $1/\sin^2 \alpha$ in Eq.(4.30b) (see also the analogous step in Eq.s(4.41) and (4.42)). In view of Eq.(4.49b), in the deformed case the factor $(1-x^2)^{l} \frac{l}{2} \Psi_{nl}(\alpha) = \sin 2l \alpha$ in $\Psi_{nl}(\alpha)$. When substituted back into Eq.(4.31a), calculation shows that only if we replace $l(l+1)$ by $2l(2l+1)$ in this
equation the denominator $1/\sin^2 \alpha$ will disappear. Next, we need to adapt the fundamental Eq.(4.34) for the Gegenbauer polynomials to $C_{n_r}^{2l+\gamma}(x)$ to our current needs. Such an adaptation produces:

$$(1 - x^2)\frac{d^2}{dx^2}C_{n_r}^\lambda(x) - (4l + 4)x\frac{d}{dx}C_{n_r}^\lambda(x) + n_r(n_r + 4l + 3)C_{n_r}^\lambda(x) = 0, \lambda = 2l + 3/2. \quad (4.52)$$

At the same time we should compare Eq.(4.52) with Eq.(4.33) in which we have to replace $l$ by $2l$. Comparison indicates that the match is achieved only if we replace $C_{n_r}^{2l+\frac{\gamma}{2}}(x)$ by $C_{n_r}^{\frac{\gamma}{2}+1}(x)$ and take $\gamma = 1/2$. The combination $\left(\sin \frac{i}{2} \alpha \right) C_{n_r}^{\frac{\gamma}{2}+1}(x)$ is fully consistent with two dimensional result, Eq.(4.47b). This is very plausible if we would like to apply the Hopf mapping to the two dimensional result, Eq.(4.47b), to get the result on $S^3$. Furthermore, under such circumstances we can repeat word-for-word the discussion following Eq.(4.34), that is if $\lambda = 2l + 1$, then $2\lambda + 1 \equiv 4l + 3$. Also, $n(n + 2\lambda) \equiv I_{nl} = 2l(2l + 2)$ implying the relationship $n + 2l + 1 = 2F + 1$. If, as before, we let $\hat{n} = n + l + 1$, then $2F + 1 = \hat{n} + l$. By analogy with the derivation of the hydrogen spectrum, Eq.(4.38), we now obtain:

$$E_n = -\frac{Z^2 e^4}{w(2F + 1)^2}, F = 0, \frac{1}{2}, 1, \ldots \text{ or, } E_n = -\frac{Z^2 e^4}{w(\hat{n} + l)^2}, w = \text{const.} \quad (4.53)$$

In arriving at Eq.(4.53) we took into consideration the scaling analysis presented in Appendix G and in section 2. We also used the Remark 5.3. of the following section. The obtained result is fully consistent with the Madelung rule and group-theoretical analysis of periodic system [1],[105] done in close analogy with the Gell-Mann-Zweig theory of quark-hadron matter. Additional details on origin and justification of the Madelung rule are given in section 5 and Appendix G.

5. Bertrand spacetimes in the atomic physics

5.1. General comments

The title of our paper involves phrase ”modified Bertrand theorem”. This terminology was introduced by Volker Perlick [23]. Perlick was interested in finding the relativistic analogue of the Bertrand theorem. That is he wanted to find all spherically symmetric and static spacetimes (in the sense of general relativity) all of whose bounded trajectories are periodic. Although Perlick succeeded in finding such spacetimes (which he calls ”Bertrand spacetimes”), he was puzzled by the fact that the metric of such spacetimes is not reduced to the Schwartzshild metric used for description of spacetimes around massive objects, e.g. of our Sun. Such a metric leads to the precession of planetary trajectories rotating around the Sun. This result was explained by Einstein using his theory of general relativity. Classical
Bertrand theorem forbids such a precession and, by design, its relativistic extension also forbids precession. 2 types of Bertrand metric found by Perlick caused Perlick to wonder about kind of a body (isolated from all other gravitational sources) that produces a metric in which all bounded trajectories are periodic. He concluded that "such a body must be a rather exotic object". The authors of [106] suggested that such a body should be identified with the dark matter. A quick introduction into this topic is given in our work [107], page 27. Further studies of dynamics in Bertrand spacetimes revealed [20] that dynamics in such spacetimes is superintegrable since the orbits are closed by design. Closure of orbits had prompted study of the quantum Bertrand systems [108], [109]. In these references no attempt was made to connect the obtained results with atomic physics. The purpose of this section is to demonstrate that the central object of our study, the D-O Eq.(3.19), justly belongs to the set of quantum Bertrand systems.

As before, this demonstration is essential to present in the proper context. Specifically, we begin with the Groenewold-van Hove (G-vH) theorem nicely explained in [110], [111]. Basically, it is telling us that only the harmonic oscillator-type dynamical systems can be unambiguously quantized. The St"ackel transform connects the harmonic oscillator with the Kepler-Coulomb systems [108]. Only these two systems are permissible by the classical Bertrand theorem and, formally, can be quantized without violating the G-vH theorem. Extension of the Bertrand theorem to curved spacetimes results in producing a class of superintegrable systems, including the Kepler-Coulomb-type [20], also quantizable [108], [109]. There are two independent ways to develop quantum mechanics without violating G-vH.

The first one is using the Morse theory for development of sophisticated asymptotic (semiclassical) methods of analysis of quantum mechanical problems [112]. The latest monograph [113] aimed at physically educated readers presents a detailed panoramic view of successful applications of semiclassical methods to all branches of quantum mechanics.

The idea of the second method belongs to Eisenhart. Although his results are summarized in section 4.3., because of their use in Perlick’s work [23], we need to add additional details at this point. These are coming from recognition of the fact that the addition of time transformations into symplectomorphisms of classical mechanics makes it effectively general-relativistic [107]. Indeed, suppose that the Lagrangian \( \mathcal{L} \) of a dynamical system is given by

\[
\mathcal{L} = T(p, q) - V(q), T(p, q) = \frac{1}{2} g_{ij}(q) v^i v^j.
\]  

(5.1)

The configuration space \( Q \) of this system is a Riemannian manifold whose metric \( ds^2 = g_{ij}(q) dq^i dq^j \) is determined by the kinetic term in Eq.(5.1). The Hamiltonian \( \mathcal{H}(q, p) \) is obtainable in a usual way as

\[
\mathcal{H}(q, p) = \tilde{T}(p, q) + V(q), \tilde{T}(p, q) = \frac{1}{2} g^{ij}(q) p_i p_j, \quad p_i = g_{ij}(q) v^j, \quad g^{ij} g_{jk} = \delta^i_k.
\]  

(5.2)

By extending the configuration space \( Q \) to \( \tilde{Q} = R \times Q \) and adding a new momentum, say, \( p_z \)
leads to the replacement of $\mathcal{H}(q, p)$ by

$$\tilde{\mathcal{H}}(q, p) = \frac{1}{2} g^{ij}(q) p_i p_j + \frac{1}{2} V(q) p_z^2. \quad (5.3)$$

Accordingly, the metric $ds^2$ changes to

$$d\sigma^2 = g_{ij}(q) dq_i dq_j + \frac{dz^2}{V(q)}. \quad (5.4a)$$

If such an extension is caused by changes of time variable making it dynamical\(^{32}\), we obtain the metric $d\sigma^2$ used in Perlick’s paper [23], e.g.

$$d\sigma^2 = g_{ij}(q) dq_i dq_j - \frac{dt^2}{V(q)}. \quad (5.4b)$$

In section 4.3 we noticed that the Eisenhart lift of a dynamical system involves the condition $\tilde{\mathcal{H}}(q, p) = 0$ essential for recovery of the original dynamics. Such a condition leads to Eq.(4.3) associated with the equation for null geodesics. Eq.(4.3) is conformally invariant\(^{33}\) Hamilton-Jacobi (H-J) equation. In spite of its simple look, the additive separation of variables\(^{34}\) is highly nontrivial. The nontriviality of separation problem in classical H-J equation leads to nontriviality of the quantization problem associated with the conformal Laplacian, Eq.(3.12). References [70], [93] illustrate the essence of this problem. Results of these references should be considered as alternative to the G-vH theorem\(^{35}\). In addition to the references just mentioned, we recommend to our readers excellent lectures by Benenti [114] as well as the thesis [115] by Bruce. Both are containing many practical examples. From Benenti lectures as well as from [93] and Appendix F it follows that the analysis of the H-J equation can be done the same way even if $\tilde{\mathcal{H}}(q, p) = E \neq 0$, e.g. for Eq.(B.16). With such a background we are ready to demonstrate that, in accord with expectations of Demkow and Ostrovsky\(^{7}\), Eq.(3.19) indeed belongs to the set of equations describing quantum Bertrand systems in the sense of \(^{108}\),c\(^{109}\).

5.2. D-O Eq.(3.19) as the benchmark example of a quantum Bertrand system

We begin by rewriting Eq.(3.19) in the equivalent form

$$\left(\frac{r}{a}\right)^2 \left[ \frac{1}{\gamma+1} (r/a) - (r/a)^{\gamma} \right]^2 \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi + n_0^2 \psi = 0 \quad (5.5a)$$

For $\gamma = 1$, that is for hydrogen atom, this equation coincides with Eq.(3.35) as required. Accounting for scaling arguments presented in Eq.(2.14), classical mechanics version of this

\(^{32}\)Section 3 and Appendix B.

\(^{33}\)Theorem 3.1.

\(^{34}\)Eq.(4.4).

\(^{35}\)Perhaps, the Bertrand-Darboux theorem should be linked with G-vH theorem in deciding which dynamical system is admitting quantization.
equation coincides with Eq.(2.29). For arbitrary \( \gamma \) classical version of Eq.(5.5) reads \((\hbar = 1, m = 1)\)

\[
\left( \frac{r}{a} \right)^2 \left[ (r/a)^{-\gamma} + (r/a)^{\gamma} \right]^2 |p|^2 = n_0^2
\]  

(5.5b)

or, in the case if \( \gamma = 1/2 \), we get

\[
\left( \frac{r}{a} \right) [1 + (r/a)]^2 |p|^2 = n_0^2 .
\]  

(5.5c)

In such a form (without applications to atomic physics) this result reads as Eq.(2.119), page 49, of the PhD thesis [108] on quantum Bertrand spaces. In Eq.(2.119) we have to put \( K = -1, \beta = \gamma, \) and \( \frac{P^2}{4} = |p|^2 \). It remains to demonstrate how this result emerges from Perlick’s results [23].

We begin with some comments on two types of metric obtained in [23]. We describe only type I metric, that is the Kepler-Coulomb (KC) type. The type II metric, the oscillator-like, is obtainable from type I via Stäckel transform as demonstrated in [108]. The type I metric is described as

\[
d\sigma^2_I = \frac{dr^2}{\beta^2(1 + Kr^2)} + r^2(d\theta^2 + \sin^2 \theta \, d\phi^2) - \frac{dt^2}{G + \sqrt{r^{-2} + K}}
\]  

(5.6)

Here \( G \) and \( K \) are some constants while \( \beta \) is rational number. By comparing Eqs. (5.3),(5.4) and letting \( G = K = 0 \) and \( \beta = 1 \) we recover the KC Hamiltonian

\[
\hat{H}_{CK} = p_r^2 + \frac{L^2}{r^2} - \frac{1}{r}.
\]  

(5.7)

In general, the associated Hamiltonian, Eq.(5.2), reads

\[
\mathcal{H}_I(q,p) = \frac{\beta^2}{2} (1 + Kr^2)p_r^2 + \frac{L^2}{r^2} - \sqrt{r^{-2} + K} + G.
\]  

(5.8)

The task now is to relate Eq.(5.5b) to Eq.(5.8). This requires several steps. The Perlick metric, Eq.(5.4b), defines the kinetic energy realized on null geodesics of 3+1 dimensional space-time of Lorentzian signature. Alternatively, it can be used for description of the motion in 3 dimensional spherically symmetric space with the metric

\[
d\Sigma^2_I = \frac{dr^2}{\beta^2(1 + Kr^2)} + r^2(d\theta^2 + \sin^2 \theta \, d\phi^2)
\]  

(5.9)

describing the classical motion on 3 manifold with metric \( d\Sigma^2_I \) in the presence of spherically symmetric potential \( V(r) \). To move forward, following [116] we need to look at several alternative ways of writing \( d\Sigma^2_I \). Specifically,

\[
d\Sigma^2_I = g(r)dr^2 + r^2d\Omega^2 = F^2(\rho)(d\rho^2 + d\Omega^2) = f(\|q\|)d|q|^2 = f^2(\tilde{r})(d\tilde{r}^2 + \tilde{r}^2d\Omega^2)
\]  

(5.10)

\[^{36}\text{Since } G \text{ is arbitrary constant thus far, we are free to change its sign.}\]
Here \( d\Omega^2 = d\theta^2 + \sin^2 \theta \, d\varphi^2 \), \( dq^2 = dq_1^2 + dq_2^2 + dq_3^2 \). \( q_1 = \tilde{r} \cos \theta \), \( q_2 = \tilde{r} \sin \theta \cos \varphi \), \( q_3 = \tilde{r} \sin \theta \sin \varphi \). \(|q| = \tilde{r}, \rho = \ln \tilde{r} \). Use of the metric written in the form \( f(|r|) \, dr^2 \) immediately brings us to Eq.(3.35). But we still can do more since our task is to relate Eq.(5.5b) to Eq.(5.8). Therefore, we have to take into account that \( f(|r|) = f(\tilde{r}) \). To determine \( \tilde{r} \) and \( f(\tilde{r}) \) we have to take into account that:

a) \( F(\rho) = \tilde{r} f(\tilde{r}) \),

b) \( \frac{d\rho}{dr} = \frac{1}{r} - \frac{1}{2} G(\tilde{r}) \)

c) \( r = F(\rho) \).

From Eq.(5.10) and just defined results we obtain:

\[
\begin{align*}
\text{a)} \quad & \frac{r}{\tilde{r}} = f(\tilde{r}); \quad \text{b)} \quad g(r) = \frac{1}{\beta} \frac{1}{\sqrt{1 + Kr^2}}; \quad \text{c)} \quad \frac{d\rho}{dr} = \frac{1}{\beta r \sqrt{1 + Kr^2}} \\
& \quad \quad (5.11)
\end{align*}
\]

Integrating Eq.(5.11c)) yields

\[
\rho = \frac{1}{\beta} \ln \left( \frac{r}{1 + \sqrt{1 + Kr^2}} \right). \quad (5.12)
\]

Since \( \rho = \ln \tilde{r} \) we obtain as well

\[
\tilde{r} = \frac{r}{1 + \sqrt{1 + Kr^2}}. \quad (5.13)
\]

Since according to Eq.(5.11a)) \( \frac{r}{\tilde{r}} = f(\tilde{r}) \), by resolving Eq. (5.13) with respect to \( r \) we obtain

\[
\left( \frac{r}{\tilde{r}} \right)^2 = f^2(\tilde{r}) = \frac{4}{\tilde{r}^2} \left( \frac{1}{r - \beta} - K\tilde{r}^\beta \right)^2. \quad (5.14)
\]

Taking into account Eqs. (5.1)-(5.4), (5.6)-(5.10) (and omitting tildas) we obtain the (null) Hamiltonian

\[
r^2(r^{-\beta} - Kr^\beta)^2 |p|^2 + \alpha = 0 \quad (5.15)
\]

Here \( K \) and \( \alpha \) are some constants. They are fixed by comparing Eq.s (5.15)and (5.5c).

This is achieved by selecting respectively \( \beta = 1/2, K = -a^{-1} \) and \( \alpha = -n_0^2 \). Thus, we just established the desired correspondence between the D-O Eq.(3.19) and the generalized Bertrand problem.

By looking at Eq.s (5.6),(5.8) and (5.10) it remains to demonstrate that presence of the potential \( -\sqrt{r^{-2} + K} + G \) in Perlick’s Hamiltonian, Eq.(5.8), is harmless for the correspondence we just established. For this purpose we need to take into account that \( \sqrt{r^{-2} + K} = \frac{1}{2}(r^{-\beta} + Kr^\beta) \). This result is obtained on page 8 of [116]. In terms of these variables the Hamiltonian, Eq.(5.8), acquires the following form

\[
\mathcal{H}_I(r,p) = \frac{1}{4} r^2(r^{-\beta} - Kr^\beta)^2 |p|^2 - \frac{1}{2} (r^{-\beta} + Kr^\beta) + G. \quad (5.16)
\]

Using the conformal Stäckel transform described in the Appendix F the Hamiltonian \( \mathcal{H}_I(r,p) \) is obtainable from \( \mathcal{H}_I(r,p) \) as follows. Relabel \( \mathcal{H}_I(r,p) \) as \( \mathcal{H}_{II}(r,p) \), where \( U = -\frac{1}{2} (r^{-\beta} + Kr^\beta) + G \). Let

\[
\mathcal{H}(r,p) = r^2(r^{-\beta} - Kr^\beta)^2 |p|^2 + \alpha. \quad (5.17a)
\]
The Hamiltonian $H_{II}(r,p)$ is defined now as

$$H_{II}(r,p) = \frac{H(r,p)}{U} = \frac{1}{2} \frac{r^2(r^{-\beta} - Kr^\beta)^2 |p|^2}{r^{-\beta} + Kr^\beta - 2G} + \frac{2\alpha}{r^{-\beta} + Kr^\beta - 2G}. \quad (5.17b)$$

By introducing new variables $r'$ and $p'$ so that $r = F(r'), p = F(p')$ with known functions $F$ and $F$ converts $H_{II}(r,p)$ into the standard form. It is obtainable with help of Perlick's oscillator-type metric, Eq.(13) of [23], using Eq.s(5.3),(5.4). Thus, by using results of subsection 4.1., we just established the correspondence between the D-O Hamiltonian $H(r,p)$ and that obtained with help of type II Bertrand metric. Since in the conformally flat spaces of constant curvature there is a Coulomb-oscillator duality [117], this duality does exist between the Bertrand spaces of types I and II. This result is supported by the following two theorems

**Theorem 5.1.** Every nondegenerate second-order quantum superintegrable system on a 3d conformally flat space is Stäckel equivalent to a superintegrable system on constant curvature space.

**Theorem 5.2.** Every superintegrable system with nondegenerate potential on 3d conformally flat space is Stäckel equivalent to a superintegrable system on either 3d flat space or on $S^3$.

**Remark 5.3.** Theorem 5.2. provides justification of the result, Eq.(4.53), obtained in previous section.

5.3. Miscellaneous. Some remaining geometrical and topological issues

5.3.1. The notion of warped product

Perlick spacetimes are, in fact, warped products. This means the following. Consider a static (spherically symmetric in Perlick’s case) spacetime $(M, dg^2)$ made of the product of spherically symmetric 3-manifold $M$ (with metric $dg^2$) and the line (time) thus making the Lorentzian warped product. The warping function $V(q)$ must be strictly positive. The projection of each timelike geodesic on a constant time leaf $M_0 = M \times \{ t_0 \}$ is a trajectory of the dynamical system with Hamiltonian, Eq.(5.3), with $p_z^2 = 1$. Thus the trajectory in Perlick’s spacetime $(M, dq^2)$ is just a projection of the timelike geodesic onto $M_0$. For more details on warping products one should consult [120],[121].

5.3.2. The notion of curling of dynamical trajectories on manifolds of different geometry and topology. Results of Kirzhnitz (with associates), Wheeler (with associate) and Kuru (with associates). Their relation to dynamical trajectories on $M_0$. 

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37E.g. read page 49 of [108].
38[118],Theorem 17.
39[119],Theorem 4.
In section 1 we mentioned work by Little [19]. In it he obtained a remarkable result. On $S^2$ there are only 3 distinct regular homotopy classes for oriented closed curves: a) those without self-intersections, b) those with just one self-intersection and, c) those with 2 self-intersections. Because the Bertrand spaces $M_0$ are spherically symmetric and, in view Theorems 5.1. and 5.2. and, of Hopf mapping, they are topologically either $S^2$ or $S^3$. Based on these observations we anticipate Little’s results to be fully enforced. This is indeed the case. In [25] Kirzhnitz (with associates) studied Newtonian dynamic of a particle of unit mass moving in the presence of the Tietz potential $40$, Eq.(G.9), under standard initial conditions. Results were parametrized in terms of the angular momentum $L$ of the particle, charge $Z$, and dimensionless distance $x = r/a$ defined with help of Eq.(G.7) of Appendix G. The obtained trajectory is described in polar coordinates with help of the equation

$$x + 1/x = \Delta + 1 + (\Delta - 1) \cos \varphi$$

(5.18a)

describing a closed curve with just one self-intersection. The observed period $T$ is described as

$$T = \frac{\pi (\Delta + 1) (3\Delta - 1)a^2}{L}.$$  

(5.18b)

Here $\Delta = \frac{Za}{L^2} - 1$. Exactly the same type of once self-intersecting closed (periodic) motion was obtained by Wheeler [14],[16] and his assistant Powers [15]. At the time of these studies the concept of Bertrand spacetime was nonexistent. Only in 2017 a systematic study of dynamical trajectories of type I (Kepler-Coulomb) Perlick systems with Hamiltonian $H_I(q,p)$, Eq.(5.8), was performed by Kuru and associates [18]. In complete agreement with previously described results, for $\beta = 1/2$ the closed trajectories were obtained with either none or one self-intersection. These are displayed respectively in Fig.5 and Fig.7 on page 3362.

5.3.3. Topology versus geometry. How the Madelung rule emerges from Fermi’s results

The content of this subsection is closely linked with results of Appendix G. Our readers are advised to consult this appendix for additional details.

We begin with Wong’s claim [123], Eq.(G.3b), that the result $n + l = (6Z)^{1/3}$ is the Madelung rule written mathematically. As noticed in the Appendix G, this result is contradictory since the factor $(6Z)^{1/3}$ is not an integer for every nonnegative $Z$. The situation can be corrected based on the work by Ivanenko and Larin [124]. These authors simplified calculations by Fermi [125] and obtained Eq.(G.4), that is

$$Z_l = \gamma(Z_l)(2l + 1)^3.$$  

(5.19)

The $Z_l$– dependent factor $\gamma(Z_l)$ is calculated iteratively for each $Z_l$. It is demonstrated in [124] that with very good accuracy the factor $\gamma(Z_l)$ can be replaced by 0.169. Using this fact Wong’s result can be rewritten as follows

$$n + l = (6Z)^{1/3} = (6 \cdot 0.169)^{1/3}(2l + 1) \simeq 1.0046(2l + 1).$$  

(5.20)

\footnote{In earlier publication [122] by the same authors more focused exposition is given.}
In atomic physics it is common to write \( n = n_r + l + 1 \). Using this result in Eq. (G.5) (or in Eq. (5.20)) we recognize that the above equation holds only if \( n_r = 0 \). From standard textbooks on quantum mechanics this result is looking suspicious. However, the results of section 4 indicate that, in fact, use of \( n_r \neq 0 \) is suspicious if calculations are made on \( S^2 \) and, via Hopf mapping, on \( S^3 \). The same conclusion follows from the group-theoretical considerations, e.g. read [89], [90], [174], [126], [127]. Instead of repeating results of these references, the same conclusion can be reached with help of topological arguments.

We begin by recalling the 2-dimensional results of subsection 4.4. Use of the conformal mapping permits us to solve the Schrödinger equation on \( R^2 \), to lift it to \( S^2 \) and, then to lift the obtained result to \( S^3 \) using Hopf mapping. In 2 dimensions the solution of the Kepler-Coulomb quantum problem is reduced to the solution of the standard rigid rotator equation and, hence, to known results. Therefore, there is no room for \( n_r \) on \( S^2 \) in Kepler-Coulomb 2d problem. Surely, it is possible to still use \( n_r \) on \( R^2 \) as it was done by Makowski [54]. Since use of \( R^2 \) (or \( S^2 \)) allows us to perform the conformal transformations straightforwardly, it comes as no surprise that the result Eq.(4.49) for the deformed wave function is not correct as explained in the subsection 4.6.1. The corrected result, Eq.(4.53), leads to the Madelung rule and allows us to use in Eq.(5.20) \( n = l + 1 \) as required. Thus, the results by Fermi [125] imply the Madelung rule. This was recognized already by Wong [123] whose analysis required a correction. Details are presented in Appendix G and, briefly, in Eq.(5.20).

The wave function \( Y_{nlm}(\alpha, \theta, \varphi) = \Psi_{nl}(\alpha)Y_{lm}(\theta, \varphi) \) is not reflecting the underlying symmetry (geometry) and topology. This could be the likely cause for the D-O to use the remnant of 3 dimensional calculations, the \( n_r \). Since using the above representation for \( Y_{nlm}(\alpha, \theta, \varphi) \) the symmetry becomes broken. Its breakage is obscuring the relationship between the results on \( S^2 \) and \( S^3 \). Considered group-theoretically, this issue is best understood following [89] and [127]. The Lie algebra \( so(4) \) (working on \( S^3 \)) is a direct product of two \( so(3) \) Lie algebras, each describing the rigid rotators with standard spectrum \( j_i (j_i + 1) \), \( i = 1 \div 2 \). The Plücker embedding condition described in Appendix E leads to the requirement: \( j_1 = j_2 \) [127]. Thus, the Lie algebra \( so(4) \cong so(3) \oplus so(3) \). This result is achieved with help of the requirement \( j_1 = j_2 \). Topologically, \( S^3 \) is obtainable in two ways: a) either by gluing 2 solid tori to each other (Heegard splitting) or b) by gluing two 3-balls pointwise to each other [128]. The last construction can be easily explained. Begin with \( S^2 \). It can be made out of 2 discs glued to each other along the disc boundaries. Consider a stereographic projection- from the 2 sphere whose equator lies in the plane. Then, the projection can be made from the Northern pole or from the Southern pole. Thus, we obtain the correspondence between the half sphere -the disc- and the plane. It is possible then to map a plane onto the half plane and the gluing of 2 half spheres -to make an \( S^2 \) - can be identified with gluing of 2 half planes along their common boundary. By extending these ideas to \( S^3 \) we have to glue together 2 half \( (R^3) \)'s along their common plane. This is exact topological equivalent of the group-theoretic condition: \( j_1 = j_2 \).

\(^{41}\)Surely, the \( su(2) \) is working of \( S^3 \). However, the \( so(4) \) of is capable of working on \( S^3 \) very much like the rotation group \( so(3) \) on \( S^2 \).

\(^{42}\)E.g.read Appendix E
It is possible to extend just obtained results. Following \cite{ref0} the wavefunction $Y_{nlm}(\alpha, \theta, \varphi)$ can be replaced by its manifestly symmetric analog. For this, use of the manifestly symmetric 4 dimensional spherical coordinates is essential. These are given by

$$
   x_1 = R \cos \xi \cos \varphi, \quad x_2 = R \cos \xi \sin \varphi, \quad x_3 = R \sin \xi \cos \eta, \quad x_4 = R \sin \xi \sin \eta
$$

(5.21)

to be contrasted with those, given by Eq.(4.7). In terms of such coordinate parametrization the eigenvalue Eq.(4.31a) acquires the following look

$$
   \hat{L}^2 Z_{nfg}(\xi, \varphi, \eta) = I_{nfg} Z_{nfg}(\xi, \varphi, \eta) \quad (4.31b)
$$

Here \cite{ref8}

$$
   Z_{nfg}(\xi, \varphi, \eta) = (2\pi)^{-1} (2n)^{\frac{3}{2}} (-1)^F g d_{gf}^F (2\xi) \exp \{i\varphi(f + g) + i\eta(f - g)\}
$$

(5.22)

and, as before, $2F + 1 = n$. The detailed description of Wigner’s coefficients $d_{gf}^F (2\xi)$ is given in \cite{ref129}.

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Appendix A. Contributions of Constantin Caratheodory to the design of absolute optical instruments

In this appendix we shall comment on the appropriate places in the remarkable book by Caratheodory “Geometrical Optics” published in Berlin in 1937 \cite{ref22}. In it, he begins with Fermat principle, Eq.(2.1), which he rewrites as

$$
   \int_{\gamma'} L'(t', x'_i \frac{dx'_i}{dt'}) dt' = \int_{\gamma} L(t, x_i \frac{dx_i}{dt}) dt + \int_{\gamma} d\Psi, \quad i = 1 \div 3.
$$

(A.1)

This equation is being interpreted as follows. The difference between the optical lengths of two curve segments $\gamma$ and $\gamma'$ that correspond to each other by means of the stigmatic map
is equal to the difference between the values of $\Psi(t, x_i)$ at the endpoints of the curve $\gamma$. This difference is then independent of the shape of the curves $\gamma$ and $\gamma'$ and depends only upon the position of their endpoints. Under such circumstances Eq.(A.1) implies that the relation

$$L'(t', x_i)\frac{dx_i}{dt'} dt' = L(t, x_i)\frac{dx_i}{dt} dt + \left( \frac{\partial}{\partial t} \Psi \right) dt + \left( \frac{\partial}{\partial x_i} \Psi \right) dx_i$$ \hspace{1cm} (A.2)

must be fulfilled identically when one replaces the old variables $t, x_i$ by the new ones

$$t' = t'(t, x_i), \quad x'_i = x'_i(t, x_i)$$ \hspace{1cm} (A.3)

so that,

$$dt' = \frac{\partial t'}{\partial t} dt + \frac{\partial t'}{\partial x_i} dx_i \quad \text{and} \quad dx'_i = \frac{\partial x'_i}{\partial t} dt + \frac{\partial x'_i}{\partial x_j} dx_j.$$ \hspace{1cm} (A.4)

Caratheodory proves then that $\frac{\partial}{\partial t} \Psi \equiv \frac{\partial}{\partial x_i} \Psi \equiv 0$ causing Eq.(A.1) to be replaced by

$$\int_{\gamma'} L'(t', x_i)\frac{dx_i}{dt'} dt' = \int_{\gamma} L(t, x_i)\frac{dx_i}{dt} dt$$ \hspace{1cm} (A.5)

We are not reproducing the proof since Eq.(A.5) was treated by Dirac whose arguments we are presenting in section 2 of the main text. Here we only notice that the map-from the object space to the image space, given by Eq.s(A.3), must be conformal. This fact causes us to bring some facts from our earlier work [3] superimposed with results of section 2. Caratheodory notices that "From a celebrated theorem of Liouville in contrast to the planar conformal maps which depend upon infinitely many constants there is only restricted class of conformal maps of three-dimensional space. It can always be represented as a sequence of transformations through reciprocal radii of an at most five spheres. It follows then that the circles and lines in object space are transformed into curves in image space that will always be either the circles or lines. Maxwell treated the simplest case of such a ray map (when one ignores a reflection) on occasion. Furthermore," Maxwell imagined the entire space to be occupied by the medium whose index of refraction is described by Eq.(2.5) of section 2. The light rays themselves are then either circular or rectilinear. One confirms this result the most simply when one recalls the equation

$$d\sigma = \frac{2ab}{b^2 + r^2} \sqrt{dx^2 + dy^2 + dz^2}, \quad r^2 = x^2 + y^2 + z^2.$$ \hspace{1cm} (A.6)

The differential $d\sigma$, which defines the optical length of a line element inside the interior of the Maxwell fish-eye, can be also interpreted as a line element in the three-dimensional boundary

---

\[43\] Discussed in our work [3], page 50, Theorem B.8.

\[44\] Caratheodory is having in mind the M"obius and Lie sphere-type transformations discussed in our work [3] on pages 38-40 and the pentaspherical transformations discussed in section 4.

\[45\] Here the emphasis is ours

\[46\] Eq.s (2.4a) and (2.4b) of the main text.
of a four-dimensional sphere of radius \( a \) that is projected stereographically onto a space of \( x, y, z \) that should be found at a distance \( b \) from the center of the projection. Explicitly,

\[
\xi = \frac{2abx}{b^2 + r^2}, \quad \eta = \frac{2aby}{b^2 + r^2}, \quad \zeta = \frac{2abz}{b^2 + r^2}, \quad \tau = \frac{b^2 - r^2}{b^2 + r^2} \tag{A.7}
\]

so that \( \xi^2 + \eta^2 + \zeta^2 + \tau^2 = a^2 \) and, reciprocally,

\[
x = \frac{b\xi}{a + \tau}, \quad y = \frac{b\eta}{a + \tau}, \quad z = \frac{b\zeta}{a + \tau}, \quad r^2 = \frac{b^2(a - \tau)}{a + \tau}. \tag{A.8}
\]

By differentiating either Eq.(A.7) or (A.8) we reobtain Eq.s(2.4a),(2.4b) of section 2. Let now \( x, y, z \) and, respectively, \( x', y', z' \) denote the stereographic projections of two opposite points \( \xi, \eta, \zeta \) (respectively, \( -\xi, -\eta, -\zeta \)) on the four-sphere, then we obtain

\[
x' = -\frac{b^2x}{r^2}, \quad y' = -\frac{b^2y}{r^2}, \quad z' = -\frac{b^2z}{r^2} \tag{A.9}
\]

implying

\[
r'r = b^2 \tag{A.10}
\]

easily recognizable as the main result defining the Möbius geometry. This is achieved when \( b^2 = r^2 = x^2 + y^2 + z^2 \) so that \( x' = -x, \ y' = -y \) and \( z' = -z \) and, finally, \( \tau = 0 \). With these results in our hands we are in the position to interpret them using either the language of Lie sphere geometry or, which is equivalent, of twistors\(^47\) By analogy with Eq.s (6.30), [21], page 30, and, in accord with Caratheodory, we obtain the great circles on the three sphere as intersection of two hyperplanes

\[
A_k\xi + B_k\eta + C_k\zeta + bD_k\tau = 0, \quad k = 1, 2. \tag{A.11}
\]

Their intersection, when projected into \( x, y, z \) space is described by

\[
D_k(x^2 + y^2 + z^2 - b^2) - 2A_kx - 2B_ky - 2G_kz = 0, \quad k = 1, 2. \tag{A.12}
\]

These equations coincide exactly with Eq.s (7.16) of [3] as required. Recall these equations had been used in [3] to establish twistor- Lie sphere geometry correspondence. In the present case, following Caratheodory, the interpretation is as follows. Eq.s (A.12) are images of the great circles on the \( S^3 \). Due to conformal property given by Eq.(A.10) the great circles on \( S^3 \) are in one-to one correspondence with great circles on \( S^2 \) \( (S^2 : b^2 = x^2 + y^2 + z^2) \) so that if for \( S^3 \) they intersect in diametrically opposite points, the same is happening in \( S^2 \). Therefore, Eq.s (A.1) and (A.5) can be interpreted as follows. The requirement \( d\Psi = 0 \) is coming from the equality of optical lengths of the corresponding curves. That is the spherical length of two diametrically opposite curve segments is the same for both curves. Having in mind additional applications mentioned in the main text, it is useful to think about just described results as follows. Suppose that there is a manifold \( M \) (Blaschke manifold) with the property that for

\(^47\)E.g. read page 41 of [3].
each point \( P \in M \) all geodesics passing through \( P \) will meet again at the conjugated point \( P \). Then, such a medium can be used as perfect optical instrument. Arthur Besse published a book entitled "Manifolds all of whose geodesics are closed" [3A1]. Blaschke conjectured that the manifolds with such a property are \( S^n \). The current status of this conjecture is described in [130] by Benjamin McKay. For the latest optical applications of geometric and topological ideas of Besse’s book, e.g., the geodesic lenses and similar devices, please, consult [131] and [132]. Results of Besse’s book are further discussed in section 5 from the point of view of Bertrand spaces. Interesting enough, another construction of Blaschke (e.g. Blaschke products) had been used in studies of gravitational lensing [133]. Gravitational lensing can be connected with the results of this Appendix as the elaboration of the discussion in section 2 of the main text indicates. The topic of photon sphere known from general relativity [134] falls also in the same category as that of Maxwell’s fish-eye [135], [136].

Appendix B. Many uses of time changes in classical mechanics

Newtonian mechanics is invariant under Galilei transformations. Such transformations assume that time is nonchangeable parameter. However, this assumption breaks down in Newtonian mechanics as soon as mathematically rigorous treatment of collisions becomes of interest. Occurring mechanical singularities typically are being treated by the appropriate time changes. Short but excellent introduction to this topic is given in Ref.[137]. The need for variable time also emerges in theory of contact transformations. For a quick introduction, please, consult Ref.[97]. In mechanics the contact 1-form \( dS \) is given by

\[
dS = \sum_{i=1}^{n} p_i dq_i - H(q_j, \{p_j\}) dt
\]

where \( \{q_j\} = [q_1,...,q_n] \), etc. For the conservative system \( E = H(q_j, \{p_j\}) \). At least in that case it is possible to treat time \( t \) and energy \( E \) as canonically conjugate variables. So, we can make the following identifications: \( t = q_{n+1}, -E = -H = p_{n+1} \). With this identification the action \( S \) can be written in the Maupertuis form

\[
S = \int \sum_{i=1}^{n+1} p_i dq_i
\]

We would like to connect this result with that discussed in the Appendix A. For this purpose consider an equality\(^{18}\)

\[
dS' - p'_i dx'_i = \rho(S,q_j,\{p_j\}) (dS - p_i dx_i)
\]

where \( \rho(S,q_j,\{p_j\}) \neq 0 \) and \( S' = \tilde{S}(S,q_j,\{p_j\}), x'_i = x_i(S,q_j,\{p_j\}), p'_i = p_i(S,q_j,\{p_j\}) \).

The equality Eq.(B.3a) is defining a contactomorphism \([97],[138],[139]\). In contact geometry one always begins with the 1-form \( \alpha = dS - p_i dx_i \) and studies groups of contactomorphisms. Clearly, the symplectic 2-form is readily obtainable via prescription: \( \omega = d\alpha = dx_i \)

\(^{18}\)Summation over repeated indices is always being assumed
These results create an impression that the contact and symplectic geometries are different in general since it is not a priori obvious that the contactomorphic transformations are isomorphic to symplectic. To shed some light on this issue, we multiply both sides of Eq. (B.3a) by new variable $\lambda \neq 0$. Then, Eq. (B.3a) acquires the following form

$$\frac{\lambda}{\rho} (dS' - p'_i dx'_i) = \lambda (dS - p dx_i).$$

(B.3b)

By introducing new notations:

$$S = x_0; \lambda = y_0, y_i = -\lambda p_i;$$
$$S' = x'_0; \frac{\lambda}{\rho} = y'_0; y'_i = -\frac{\lambda p_i}{\rho}$$

it is possible to rewrite Eq. (B.3.b) equivalently as

$$y'_0 dx'_0 + y'_i dx'_i = y_0 dx_0 + y_i dx_i.$$  \hspace{1cm} (B.4)

Using this result along with Eqs. (B.1), (B.2) it should be obvious that Eq. (B.4) is exactly the same as Eq. (A.2) (with $\Psi = 0$) implying Eq. (A.5) and, hence, the Dirac theory of constraints, and time changes discussed in section 2. We would like to do more in this appendix.

First, we want to emphasize the differences between the contact and symplectic geometries. The major difference between these two geometries takes place when they are confronted with the description of dynamical systems subject to the constraint $H = E$. At the quantum level this topic is discussed in the Appendix F.

As soon as we are having such a constraint, the choice between two geometries is broken in favor of contact geometry. The equation $H(\{q_j\}, \{p_j\}) = E$ defines the hypersurface $\Sigma$ of dimension $2n - 1$ in $2n$ dimensional symplectic phase space $M$. To relate the vector fields on $\Sigma$ and $M$ the concept of Liouville vector field $Y$ is essential. Given that the Lie derivative $L_Y$ is defined via

$$L_Y = d \circ i_Y + i_Y \circ d,$$

(B.5)

where $d$ is the exterior differential and $i_Y$ is the contraction (both applied to differential forms $\omega$), the Liouville vector field $Y$ is defined with help of the equation

$$L_Y \omega = \omega.$$  \hspace{1cm} (B.6)

Based on this definition, the vector field $Y$ can be defined, for example, as $Y = p_i \frac{\partial}{\partial p_i}$.

The Liouville vector field $Y$ connects the symplectic and contact geometries with help of the equation

$$\alpha = i_Y \omega.$$  \hspace{1cm} (B.7)

At the same time, in symplectic geometry there is a Hamiltonian vector field $X_H$ such that

$$i_{X_H} \omega = -dH \text{ or } \omega (X_H, -) = -dH(-).$$  \hspace{1cm} (B.8a)
Here \( dH = \frac{\partial H}{\partial x_i} dx_i + \frac{\partial H}{\partial p_i} dp_i \) implying

\[
X_H = \frac{\partial H}{\partial p_i} \partial x_i - \frac{\partial H}{\partial x_i} \partial p_i
\]

since \( \omega = dx_i \land dp_i \). With such definition of \( X_H \) we obtain

\[
\omega(X_H, X_H) = -dH(X_H) = 0
\]

as required. Consider now what will happen to \( \mathcal{L}_{X_H} \omega \). Using Eq.(B.5) we obtain

\[
\mathcal{L}_{X_H} \omega = d \circ i_{X_H} \omega + i_{X_H} \circ d \omega = 0
\]

since \( d \omega = 0 \) and, because \( i_{X_H} \omega = -dH \), we also have \( d \circ i_{X_H} \omega = 0 \). Thus, the Lie derivative of the Hamiltonian vector field \( X_H \) preserves the symplectic two-form \( \omega \). The question emerges: what vector field preserves the contact form \( \alpha \)? Let us denote this field as \( R_\alpha \), so that

\[
\mathcal{L}_{R_\alpha} \alpha = d \circ i_{R_\alpha} \alpha + i_{R_\alpha} \circ d \alpha = 0.
\]

The Reeb vector field \( R_\alpha \) is defined as the field that obeys two conditions:

\[
i_{R_\alpha} \alpha = \text{const}, \quad i_{R_\alpha} \circ d \alpha = 0.
\]

Typically in literature one encounters the condition, \( \text{const} = 1 \), but it is clear that one can choose as well the condition \( \text{const} > 0 \). The question of central importance is the following

**Is there any connection between \( X_H \) and \( R_\alpha \)? and, if there is, how to describe such a connection?**

We begin with the observation [97],[138], that the very same manifold M has both the symplectic and the Riemannian structure. The Riemannian structure is described in terms of the metric tensor 2-form: \( g = g_{ij} dx^i \otimes dx^j \). Introduce now the (musical) \( \flat - \) operator converting the vector field \( X = X^i \partial_i \) into 1-form \( X^\flat = i_X g \). Introduce also the inverse operator \( \sharp \) via \( (X^\flat)^\sharp = g^{ij} X_i \frac{\partial}{\partial x^j} = X \). Suppose now that instead of Eq.(B.7) we can write

\[
\alpha = i_X g.
\]

Suppose that some vector field \( X = \tilde{X} \) is Reeb-like, that is, looking at Eq.(B.11) we have to require

\[
i_{\tilde{X}} \alpha = i_{\tilde{X}} i_{\tilde{X}} g = 1.
\]

Explicitly,

\[
i_{\tilde{X}} [g_{ij} \tilde{X}^i dx^j] = g_{ij} \tilde{X}^i \tilde{X}^j = 1.
\]

But, since \( \alpha = i_{\tilde{X}} g \) we also must have

\[
\alpha = i_{\tilde{X}} g = i_Y \omega.
\]
In view of Eq.s(B5-B7) it should be clear that $d \circ i_Y \omega = \omega$. Accordingly, in view of Eq.(B.14) we also should have $d \circ i_X g = da$. If $\tilde{X}$ is Reeb-like, then we have to have $i_X \circ da = 0$. But

$$i_X \circ da = \omega(\tilde{X}, -) = -dH(-)$$  \hspace{1cm} (B.15)

And this result becomes the same as Reeb’s 2nd condition, Eq.(B.11), only when $dH \equiv 0$. Fortunately, this is the case. This follows from the observation that Eq.(B.13b) can be reinterpreted as an equation for the Jacobi-Maupertius Hamiltonian $\tilde{H}$ for the fixed energy surface $H - E = 0$, [139]. That is

$$\tilde{H} = \frac{1}{2} \tilde{g}^{ij}(x) p_i p_j = 1,$$  \hspace{1cm} (B.16)

where

$$\tilde{g}^{ij}(x) = \frac{g^{ij}(x)}{m[E - U(x)]} \text{ or } \tilde{g}_{ij}(x) = m[E - U(x)] g_{ij}(x).$$

Alternatively, the results can be rewritten in the Lagrangian form as follows

$$\tilde{L} = \frac{1}{2} \tilde{g}^{ij}(x) \xi^i \xi^j \equiv \frac{1}{2} < \xi^i, \xi^j > = 2$$  \hspace{1cm} (B.17)

where $\xi^i = \frac{dx^i}{d\sigma}$ and $p_i = \tilde{g}_{ij}(x) \xi^j$. The Euler- Lagrange equations obtainable with Lagrangian $\tilde{L}$ are equations for geodesics [139],[35] relative to the metric $\tilde{g}_{ij}(x)$. Equations for geodesics do not change if we replace $\tilde{L}$ by $\tilde{L} = \sqrt{\tilde{L}}$. But this Lagrangian leads to the reparametrization-invariant action and is homogenous of the first degree in $\xi^i$. That is $\tilde{L}(x, \lambda \xi) = \lambda \tilde{L}(x, \xi)$.

Use of Euler’s theorem produces then: $\xi^i \frac{\partial \tilde{L}}{\partial \xi^i} = \tilde{L}$. From here we obtain the Hamiltonian

$$H = \xi^i \frac{\partial \tilde{L}}{\partial \xi^i} - \tilde{L} \equiv 0.$$ 

Thus, the Reeb vector field $\tilde{X}$ *always* describes the (null) geodesics of energy $E = 0$ in Riemannian space with metric $\tilde{g}_{ij}(x)$.

Obtained result is in agreement with that obtained by a very different set of arguments in [140], page 27. Now we are in the position to formulate the following (e.g. read [140], page 25):

**Theorem B.1.** If a codimension 1 submanifold $M$ is both a hypersurface of contact type (that is with $\alpha = i_Y \omega$) and the level set of a Hamiltonian $H$, then the Reeb flow

is reparametrization of the Hamiltonian flow.

**Proof:** on one hand we have $i_{R_a} \circ da \mid_{\Sigma} = 0$, on another hand, we have $i_{\tilde{X}} \circ da \mid_{\Sigma} = \omega(\tilde{X}, -) \mid_{\Sigma} = -dH(-) \mid_{\Sigma} = 0$.

Obtained results still requires some improvement. Let us return to the 1-form $\alpha = dS - p_i dx^i$ defined after Eq.(B.3a). A contact structure on a manifold $M$ of odd dimension
(say, $2n+1$) is a hyperplane field $\zeta = \ker \alpha$ such that $\alpha \wedge (d\alpha)^n \neq 0$. The pair $(M, \zeta)$ is called **contact manifold** [97],[140]. Now, notice that $\ker \alpha$ is known in mechanics as a statement: $p_i = \partial S/\partial x_i$. Thus, the action $S = S(\{x_i\})$ is a surface for which $\omega = dx_i \wedge dp_i = 0$. Such surfaces are called **Lagrangian surfaces**. On Lagrangian surfaces the Bohr-Sommerfeld quantization condition reads: $\int p \, dx = 0$. The infinitesimal automorphisms of $\zeta = \ker \alpha$ are also described in terms of the vector fields. Suppose that $\tilde{X}$ introduced after Eq.(B.12) is one of these fields. Then, Eq.(B13b) can be equivalently rewritten as $\alpha(\tilde{X}) = 1$. But we already know from Eq.(B.16) that $\tilde{H} = 1$. Therefore we can write $\alpha(\tilde{X}) = \tilde{H}(\tilde{X})$ so that $\tilde{H}(\tilde{X})$ defines now the **contact Hamiltonian**. Unlike the Liouville vector field for which Eq.(B.6) holds, it makes sense to require

$$L_{\tilde{X}} \alpha = \mu \alpha$$

(B.18)

to be compared with Eq.(3.22). The physical meaning of $\mu$ multiplier is to be determined momentarily. For this purpose we follow [141], page 57. According to this reference for the Hamiltonian $H$ we should discuss the dynamics under constraint: $H = c$. Suppose that initially such a Hamiltonian is used for description of dynamical system described by

$$\frac{dx}{dt} = H_y(x,y), \quad \frac{dy}{dt} = -H_x(x,y).$$

(B.19a)

Changing time

$$s = \int_0^t d\tau \lambda(\phi^\tau(x,y)) \quad \text{or} \quad \frac{ds}{d\tau} = \lambda$$

(B.19b)

converts the equations of motion into the following form:

$$\frac{dx}{dt} = \lambda^{-1}(x,y)H_y(x,y), \quad \frac{dy}{dt} = -\lambda^{-1}(x,y)H_x(x,y).$$

(B.19c)

This causes the Hamiltonian Eq.s(B.19a) to loose their Hamiltonian form. Nevertheless the function $\tilde{H} = \lambda^{-1}(H - c)$ can be taken as new (actually contact) Hamiltonian on hypersurface $H = c$ where

$$d\tilde{H} = \lambda^{-1}dH$$

(B.20)

Accordingly, for the vector fields on such hypersurface, $X_{\tilde{H}} = \lambda^{-1}X_H$. Earlier we obtained: $\alpha(\tilde{X}) = \tilde{H}(\tilde{X})$. Therefore, in view of Eq.(B.5), Eq.(B.18) can be rewritten now as

$$d\tilde{H} = i_{\tilde{X}} d\alpha = \mu \alpha$$

(B.21)

This result was obtained with help Eq.s(B.13) and (B.16). Taken on the Reeb vector field $R_\alpha$, this equation becomes: $d\tilde{H}(R_\alpha) = \mu$. By rewriting Eq.(B.21) as

$$d\tilde{H}(R_\alpha)\alpha - d\tilde{H}(\tilde{X}) = i_{\tilde{X}} d\alpha$$

(B.22a)

and, since $\tilde{X}$ is Reeb-like, we get $i_{\tilde{X}} d\alpha = 0$ causing us to arrive at the final (equivalent) form of Eq.(B.20), that is $d\tilde{H} = \mu \alpha$
Appendix C. Some auxiliary facts about conformal motions

Although there is a number of good sources on this topic, e.g. [61],[62]. For the sake of uninterrupted reading, we present in this appendix some essentials.

In particular, let $x$ and $x'$ be two different points of the Riemannian manifold $M_d$ of dimension $d$. Typically, the manifold $M_d$ is covered by a system of charts. To avoid complications, we shall only consider $x$ and $x'$ placed in just one chart. Then, the equation

$$g_{ij}(x) = \frac{\partial x'^k}{\partial x^i} \frac{\partial x'^l}{\partial x^j} g_{kl}(x')$$

relates the components $g_{ij}(x)$ and $g_{kl}(x')$ of the metric tensor at points $x$ and $x'$ of $M_d$. Suppose that for $\varepsilon \ll 1$ we have

$$x'^i = x^i + \varepsilon \xi^i(x),$$

then the Killing vector field $X$ is defined by

$$X = \xi^i(x) \frac{\partial}{\partial x^i}.$$  

Substituting of Eq.(C.2) into Eq.(C.1), Taylor expanding and keeping only the 1st order in $\varepsilon$ terms results in the Killing Eq.(3.21) of the main text. Explicitly,

$$\nabla_i \xi_j + \nabla_j \xi_i = 0.$$  

Here $\xi_i = \xi^j g_{ji}$ and the covariant derivative $\nabla_i \xi_j$. It is defined as usual by

$$\nabla_i \xi_j = \partial_i \xi_j - \Gamma^k_{ij} \xi_k.$$  

Familiar isometries are translations and rotations. For $d$-dimensional space these can be represented by the $d \times d$ matrices decomposable into diagonal $d$-dimensional matrix and skew symmetric $d \times d$ matrix having $\frac{d^2 - d}{2}$ components. Thus, in the case of isometries there are $\frac{d^2 - d}{2} + d = \frac{d(d+1)}{2}$ isometry generators. There is a very important theorem by Eisenhart [66],Chr.6, which reads as follows

**Theorem C.1.** Isometric group of motion for $M_d$ can have no more than $\frac{d(d+1)}{2}$ elements. The maximum number is achieved only for spaces of constant scalar curvature.

For description of these spaces we follow the classical book by Petrov [53]. In chapter 1 of this reference we find the following

**Theorem C.2.** In order for $M_d$ to be a space of constant curvature it is necessary and sufficient that the Riemannian curvature tensor $R_{ijkl}$ can be represented in the form

$$R_{ijkl} = K(g_{ik}g_{jl} - g_{jk}g_{il}).$$
where $K$ is constant.

Eq.(C.6) is satisfied if the metric can be presented in the form

$$ds^2 = \frac{1}{\sigma^2} \sum_{i=1}^{d} \varepsilon_i (dx^i)^2$$  \hspace{1cm} (C.7)

where $\varepsilon_i = \pm 1$ are in accord with the signature of $\mathcal{M}_d$ and, the conformal factor $\sigma$ is determined based on Eq.(C.6) and known definition of $R_{ijkl}$ via Christoffel’s symbols. This leads to the following set of equations

$$\partial_{ij} \sigma = 0, \sigma [\varepsilon_i \partial_{jj} \sigma + \varepsilon_j \partial_{ii} \sigma] = \varepsilon_i \varepsilon_j [K + \sum_{i=1}^{d} \varepsilon_i (dx^i)^2], i \neq j.$$  \hspace{1cm} (C.8)

The solution of these equations is

$$\sigma = 1 + \frac{K}{4} \sum_{i=1}^{d} \varepsilon_i (dx^i)^2.$$  \hspace{1cm} (C.9)

**Corollary C.3.** In view of Definition 3.4. and of Eq.s(C.7), (C.9), all spaces of constant curvature are conformally flat.

**Appendix D. Calculation of Christoffel’s symbols and related things**

For the metric tensor in the form $g^{ij}(x) = \rho(x)\delta^{ij}$ (or $g_{ij}(x) = \frac{1}{\rho(x)}\delta_{ij}$) calculation of Christoffel’s symbols proceeds as follows.

$$\Gamma^{i}_{kl} = \frac{1}{\rho} \delta^{ij} [ \delta_{kj} \left( \frac{\partial}{\partial x^l} \rho \right) + \delta_{ij} \left( \frac{\partial}{\partial x^k} \rho \right) - \delta_{kl} \left( \frac{\partial}{\partial x^j} \rho \right)]$$

$$= \frac{1}{2\rho} [ \delta^{i}_{k} \left( \frac{\partial}{\partial x^j} \rho \right) + \delta^{j}_{i} \left( \frac{\partial}{\partial x^k} \rho \right) - \left( \frac{\partial}{\partial x^i} \rho \right) \delta^{ij} \delta_{kl}].$$  \hspace{1cm} (D.1)

From here, in view of Eq.(3.29a), we obtain:

$$g^{kl} \Gamma^{i}_{kl} = -\frac{1}{2}[\delta^{il} \left( \frac{\partial}{\partial x^k} \rho \right) + \delta^{lk} \left( \frac{\partial}{\partial x^k} \rho \right) - d \left( \frac{\partial}{\partial x^i} \rho \right) \delta^{ij}] = \frac{d-2}{2} \delta^{ij} \left( \frac{\partial}{\partial x^j} \rho \right)$$  \hspace{1cm} (D.2)

Using Eq.(3.29a) and selecting sign “+” we obtain for covariant components of the vector $b^i$

$$b_i = a_i - \frac{d-2}{2} \frac{\partial}{\partial x^i} \ln \rho.$$  \hspace{1cm} (D.3a)
In view of Eq. (3.44) we need to consider as well the sign ",-" resulting in
\[ b_i = a_i + \frac{d - 2}{2} \frac{\partial}{\partial x^i} \ln \rho. \]  
(D.3b)

But after Eq. (3.27b) we obtained for the contravariant components of \( b^i \) the following transformation law: \( b'^i = b^i + 2g^{ij}\theta_j \). Written in the covariant form this relation looks as
\[ b'_i = b_i + 2\theta_i. \]  
(D.4)

Since the identically nonzero vector \( a_i \) always can be represented as
\[ a_i = \frac{\partial}{\partial x^i} \psi, \]  
(D.5)

it is possible by combining Eq. s(D.3b) and (D.4) to represent vector \( b'_i \) as
\[ b'_i = \frac{\partial}{\partial x^i} [\psi + \frac{d - 2}{2} \ln \rho + 2\theta]. \]  
(D.6)

From here, it follows that if in Eq. (3.27a) the transformation is performed with
\[ \theta = \frac{d - 2}{4} \ln \rho - \frac{1}{2} \psi, \]  
(D.7)

the transformed Eq. (3.27b) will have \( b'^i = 0, i = 1, ..., d \). In calculating of Eq. (3.37) we needed to evaluate \( \Gamma^i_{ki} \). In view of Eq. (D.1), this can be done as follows.
\[ \Gamma^i_{ki} = -\frac{1}{2\rho} (\rho_i \delta^i_k + \rho_k \delta^i_i - \rho_j \delta^{ij} \delta_{ki}) = -\frac{d \rho_k}{2 \rho}. \]  
(D.8)

**Appendix E. Solution of the constraint Eq. (4.29).**

**SO(4) rotational group and Plücker matrices**

In this appendix we are discussing the role of the constraint, Eq. (4.29), in finding solutions of Eq. (4.26b). This equation is obtained by mapping the 3 dimensional Schrödinger’s Eq. (3.19a) with potential Eq. (3.19b) (\( \gamma = 1 \)) onto \( S^3 \). We need to demonstrate that the constraint, Eq. (4.29), is enforcing the spherical topology of \( S^3 \).

We begin with using some results from our work [3]. Specifically, in section 6 of [3] we defined the moment \( L \) and the Laplace-Runge-Lentz vector \( A \) for the hydrogen atom model Hamiltonian. These vectors are subject to the 3-dimensional constraint: \( L \cdot A = 0 \). To connect this result with Fock’s results on hydrogen atom [89], we found in [3] that it is convenient to look at this constraint from the point of view of the 4-dimensional space. Both in 3 and 4 dimensions this equation represents the Plücker embedding condition. Because of this, the constraint, Eq. (4.29), is of the same category as previously studied constraint \( L \cdot A = 0 \).

Quantization of \( L \) and \( A \) leads to 2 decoupled \( \text{so}(3) \) Lie algebras as demonstrated in [3].
and [89]. From group theory [89] is is known that the Lie algebra $\mathfrak{so}(4) \cong \mathfrak{so}(3) \oplus \mathfrak{so}(3)$. This observation is the starting point of our analysis.

Let the vector $X \in \mathbb{R}^4$ be described as $X = [U,V,W,T]^T$. Using this notation we consider all points $X \in \mathbb{R}^4 \setminus \{0\}$. They can be used for design of projective space $\mathbb{P}^3$. It can be constructed out of equivalence classes made out of vectors $X$ and $Y \in \mathbb{R}^4 \setminus \{0\}$ such that $X = \lambda Y$, $\lambda \neq 0$. To distinguish between the $\mathbb{R}^4$ and $\mathbb{P}^3$ the homogenous coordinates should be introduced, e.g. via notation: $X = [U:V:W:T]$. This helps us to identify the points of $\mathbb{P}^3$ with the equivalence classes. Clearly, the 3 dimensional vectors, e.g. $v$, are obtained now as $v = [U^T, V^T, W^T]^T$.

Reciprocally, a homogenous presentation of the 3-vector $v = [U,V,W]^T$ is given by $v = [U:V:W:1]$. Thus, $\mathbb{P}^3$ is made of all points $[U,V,W]^T$ of $\mathbb{R}^3$ plus the points $[U:V:W:0]$ at infinity comprising a projective plane $\mathbb{P}^2$. Planes in $\mathbb{P}^3$ can be defined with help of the concept of duality defined with help of the scalar product $<,>$ in Euclidean space. Specifically, consider the equation

$$< \pi, X > = \pi_1 X_1 + \pi_2 X_2 + \pi_3 X_3 + \pi_4 X_4 = 0. \quad (E.1a)$$

It is looking exactly the same as Eq.(4.29). Its interpretation is the following. The point $X = [X_1:X_2:X_3:X_4]$ lies on the hyperplane $\pi = [\pi_1:\pi_2:\pi_3: \pi_4]$ if and only if Eq.(E.1a) is satisfied. Thus, in projective spaces the planes and the points are equivalent in view of the duality just defined. Clearly, in a more familiar 3 dimensional setting the same result is presented as

$$\pi_1 X + \pi_2 Y + \pi_3 Z + \pi_4 = 0, \quad (E.1b)$$

where $X=X_1/X_4, Y=X_2/X_4, Z=X_3/X_4$. Eq.(E.1a) can be conveniently rewritten as

$$\pi^T X = 0. \quad (E.1c)$$

Because of the duality, there is a compelling reason to look as well at the equation

$$\begin{bmatrix}
X_1^T \\
X_2^T \\
X_3^T \\
X_4^T 
\end{bmatrix} \pi = 0. \quad (E.2a)$$

This should be understood as follows. Three points $X_1, X_2, X_3$ in general position define a plane. Each of these points is satisfying Eq.(E.1c), that is, $\pi_i^T X_i = 0, i = 1 \div 3$. Therefore, Eq.(E.2) is defining a plane determined by 3 prescribed points in general position. Using duality, we also get

$$\begin{bmatrix}
\pi_1^T \\
\pi_2^T \\
\pi_3^T 
\end{bmatrix} X = 0. \quad (E.2b)$$

To proceed, we need to define the notion of a line in $\mathbb{P}^3$ and to connect it with the results pertinent to the Lie algebra $\mathfrak{so}(4)$. In doing so, we follow the original Plücker ideas described in [3] and [97]. Some results from lecture notes by William Goldman [143] are also helpful.
Specifically, we need to recall that the Lie algebra $\mathfrak{so}(4)$ is made out of the set of $4 \times 4$ skew-symmetric matrices. These can be built as follows

$$\mathbb{R}^4 \times \mathbb{R}^4 \rightarrow \mathfrak{so}(4) \text{ or, explicitly, } (\mathbf{v}, \mathbf{w}) \rightarrow \mathbf{v} \wedge \mathbf{w} := \mathbf{wv}^T - \mathbf{v}\mathbf{w}^T := \mathbf{L}. \quad (E.3)$$

Here $\mathbf{L}$ is defining the Plücker matrix describing the line $l$ in $\mathbb{P}^3$. The notion of Plücker matrix is absent in [3], [97] and [142]. It is essential, however, and requires some explanation.

To do so, we follow Plücker’s ingenuous idea that 3 dimensional lines can be described in terms of 3 dimensional vectors $\mathbf{y}$ and $\mathbf{x}$, taken from the same origin $\mathbf{o}$, whose ends are located on the line $l$. In 3-space the direction for such a line is $\mathbf{r} := \mathbf{y} - \mathbf{x}$. The shortest distance $\mathbf{z}$ between $l$ and $\mathbf{o}$, the cross product $\mathbf{n} = \mathbf{y} \times \mathbf{x}$ and $\mathbf{r}$ are forming the right handed tripod. Any 2 of these 3 vectors are sufficient to determine the 3rd one. Typically the vectors $\mathbf{r}$ and $\mathbf{n}$ are chosen. With these results in our hands, following Plücker, we introduce

$$p_{01} = y_1 - x_1; \quad p_{23} = x_2 y_3 - x_3 y_2, \quad (E.4a)$$
$$p_{02} = y_2 - x_2; \quad p_{31} = x_3 y_1 - x_1 y_3, \quad (E.4b)$$
$$p_{03} = y_3 - x_3; \quad p_{12} = x_1 y_2 - x_2 y_1. \quad (E.4c)$$

From these results it follows that $\mathbf{x} = (x_1, x_2, x_3)^T, \mathbf{y} = (y_1, y_2, y_3)^T, p_{ij} = x_i y_j - x_j y_i, x_0 = y_0 = 1$. The Plücker relation, Eq.(6.18c), of [3] in terms of just defined notations acquires the form $\mathbf{n} \cdot \mathbf{r} = 0$, where

$$\mathbf{r} = \begin{bmatrix} p_{01} \\ p_{02} \\ p_{03} \end{bmatrix} \text{ and } \mathbf{n} = \begin{bmatrix} p_{23} \\ p_{31} \\ p_{12} \end{bmatrix}^T.$$

Explicitly,

$$p_{01}p_{23} + p_{02}p_{31} + p_{03}p_{12} = 0. \quad (E.5)$$

Suppose now that $\mathbf{q}$ is the point lying on the line $l$ determined by $\mathbf{n}$ and $\mathbf{r}$. Then, the condition that the point $\mathbf{q}$ is indeed lying on the line $l$ is given by

$$\mathbf{r} \times \mathbf{q} = \mathbf{n}. \quad (E.6)$$

To prove this, we assume that $\mathbf{q} = \mathbf{y} + \lambda \mathbf{r}$ where $\lambda$ is some nonzero arbitrary multiplier. By substituting this result into Eq.(E.6) we indeed obtain the identity. Next, we need to convert this result into manifestly 4 dimensional form. This can be achieved as follows. We begin with representation for the Lie algebra $\mathfrak{so}(3)$. A suitable basis is made out of matrices $(\mathcal{A}_i)_{jk} = -\epsilon_{ijk}$. Here $i, j$ and $k$ can take values $1 \div 3$. To generalize this result to $\mathfrak{so}(4)$, it is convenient to begin with

$$(\mathcal{A}_1)_{jk} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (\mathcal{A}_2)_{jk} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (\mathcal{A}_3)_{jk} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (E.7)$$
These matrices obey the so(3) commutation relations \([A_i, A_j] = \epsilon_{ijk} A_k\). Using just defined matrices, we can now define the \(B\)-matrices also obeying the same commutator algebra \([B_i, B_j] = \epsilon_{ijk} B_k\). Thus, we obtain so(4) \(\cong\) so(3) \(\oplus\) so(3). This is the Lie algebra of hydrogen atom [3], [89]. Explicitly, the \(B\) matrices are given by

\[
(B_1)_{jk} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},
(B_2)_{jk} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},
(B_3)_{jk} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}
\]  
(E.8)

By looking at Eq.(E.3) we consider now designing of a specific line- the X axis. It can be constructed using 2 reference points

\[
\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = w \text{ and } \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = v
\]

representing the origin of X-axis and the point at infinity for the X axis. Following Eq.(E.3), we obtain now for the X-line the following result:

\[
L = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} - \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} = (B_1)_{jk}.
\]  
(E.9)

Just obtained result allows us to rewrite Eq.(E.6) in 4 dimensional form

\[
\begin{pmatrix} 0 & p_{23} & -p_{13} & p_{12} \\ -p_{23} & 0 & p_{03} & -p_{02} \\ p_{13} & -p_{03} & 0 & p_{01} \\ -p_{12} & p_{02} & -p_{01} & 0 \end{pmatrix} \begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix} = 0
\]  
(E.10)

The correctness of this result is easily checked following [143], page 201. From this reference we find

\[
x \times y = \begin{pmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}.
\]  
(E.11)

The 4 dimensional extension of this result is straightforward. Evidently, the result, Eq.(E.10), coincides with the constraint, Eq.(4.29). However from Eq.(4.26b) it follows that there are 4 momenta while we just got 6 vectors since every so(4) matrix is decomposable in terms of the 6 skew-symmetric matrices \(A_i\) and \(B_i\). To clarify this mismatch, we follow [3] and [142]. In \(\mathbb{R}^4\) we are having \(\{e_0, ..., e_3\}\) as the basis. Using this basis we can construct the set of exterior products. To label these products we need to define the subsets \(J_p = \{i_1, ..., i_p\}, p \leq n\). There

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are exactly \( n!/(n-p)!p! \) of such subsets. Change of the basis: \( \{ e_0, ..., e_n \} \) to \( \{ e'_0, ..., e'_n \} \) leads to projective equivalence, e.g. to \( e'_{i_1} \wedge \cdot \cdot \cdot \wedge e'_{i_p} = \text{det}(A_{ij})e_{i_1} \wedge \cdot \cdot \cdot \wedge e_{i_p}. \) The Grassmannian \( \text{Gr}_p(\mathbb{R}^n) \) is made out of all of just defined \( p \) -dimensional subspaces of \( \mathbb{R}^n \). Let \( n=4 \) and consider all 2 dimensional subspaces of \( \text{Gr}_2(\mathbb{R}^4) \). These are made of 2-planes, e.g. \( e_i \wedge e_j \). There are \( 6 = 4!/2!2! \) planes which replace the 4 basis vectors \( \{ e_0, ..., e_3 \} \). Because of the projective equivalence of such planes, they are Plücker embedded into 5 dimensional projective space \( \mathbb{P}^5 \). From Eqs.(E.4a-c) it is possible to establish 1-1 correspondence between the 6 planes set \( e_i \wedge e_j \) and the 6 planes set \( p_{ij} \). But \( p_{ij} \) are the momenta! The first of them, the \( p_0 \), is made out of planes \( e_0 \wedge e_1, e_0 \wedge e_2, e_0 \wedge e_3 \). There are 3 \( so(4) \) matrices associated with these planes. The second- the \( p_1 \), is made of planes \( e_1 \wedge e_2 \) and \( e_1 \wedge e_3 \) and the associated with them \( so(4) \) matrices and, the 3rd, the \( p_2 \), is made out of plane \( e_2 \wedge e_3 \) and the associated with it \( so(4) \) matrix. These arguments explain the mismatch. The 6 infinitesimal generators obtained with help of 6 \( so(4) \) matrices are obtainable in exactly the same way as 3 generators for the 3 dimensional rigid rotator. Their explicit form is given in Appendix C of [89].

Appendix F. Essentials of the Sturmian problem and of the conformal Stäckel transform

In our exposition of this topic we follow [70],[93],[144],[145]. In particular, following [145] we begin with brief discussion of the Sturmian problem. The hydrogen orbitals satisfy the 1-electron stationary Schrödinger equation (in the appropriately chosen system of units)

\[
[-\frac{1}{2}\nabla^2 - \frac{Z}{r} + \frac{Z^2}{2n}]\psi_{nlm}(x) = 0
\]  

(F.1a)

Denote \( k = \frac{Z}{n} \), and rewrite Eq.(F.1a) using just introduced notation:

\[
[-\frac{1}{2}\nabla^2 - \frac{nk}{r} + \frac{k^2}{2}]\tilde{\psi}_{nlm}(x) = 0.
\]  

(F.1b)

The eigenfunctions \( \tilde{\psi}_{nlm} \) obey the isoenergetic Sturmian (Schrödinger) equation:

\[
[-\frac{1}{2}\nabla^2 + \frac{k^2}{2}]\tilde{\psi}_{nlm}(x) = \beta_n \frac{1}{r} \tilde{\psi}_{nlm}(x).
\]  

(F.1.c)

In this equation, the energy \( E = -\frac{k^2}{2} \) is fixed and the eigenvalue \( \beta_n \) is \( \beta_n = nk \). If the eigenfunctions \( \psi_{nlm}(x) \) are orthogonal, i.e.

\[
\int d^3x \psi^*_{n'l'm'}(x)\psi_{nlm}(x) = \delta_{n'n}\delta_{l'l}\delta_{m'm}
\]  

(F.2a)

, the eigenfunctions \( \tilde{\psi}_{nlm}(x) \) are weighted orthogonal, i.e.

\[
\int d^3x \tilde{\psi}^*_{n'l'm'}(x) \left( \frac{n}{kr} \right) \tilde{\psi}_{nlm}(x) = \delta_{n'n}\delta_{l'l}\delta_{m'm}.
\]  

(F.2b)

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The conformal Stäckel transform following [70],[93] can be defined as follows. Begin with the manifestly conformal (Laplace-type) equation
\[ H \Psi = \left[-\frac{1}{\lambda(x)} \nabla^2 + V(x)\right] \Psi = 0. \] (F.3)
In this equation let \( V(x) = W(x) - U(x)E \). In accord with Eq.(F.1b) we shall consider the parameter \( E \) as fixed. The potential \( U(x) \) defines the conformal Stäckel transform: from manifestly conformal Eq.(F.3) (e.g. read section 3) to the Helmholtz-type equation
\[ \tilde{H} \tilde{\Psi} = E \tilde{\Psi}, \] (F.4)
where
\[ \tilde{H} = -\frac{1}{\tilde{\lambda}(x)} \nabla^2 + \tilde{V}(x). \] (F.5)
Here \( \tilde{\lambda}(x) = \lambda U, \tilde{V} = \frac{W(x)}{U(x)} \). The choice of the potential \( U(x) \) is nontrivial. It is determined by the Bertrand-Darboux system of partial differential equations.

**Theorem F.1.** Any second order conformal (Laplace-type) superintegrable system admitting nonconstant potential \( U(x) \) can be Stäckel-transformed to a Helmholtz superintegrable system. This operation is invertible. The inverse mapping is taking true symmetries to conformal symmetries.

**Remark F.2.** The nontriviality of the potential \( U(x) \) is coming from the fact that it is obtainable as a solution of the system of second order (conformal) Bertrand-Darboux (B-D) partial differential equations (PDE).

**Remark F.3.** Solutions of the B-D system of PDE’s resulting in obtaining of \( U(x) \) is linked with solution of the Bertrand problem in curved spacetimes (e.g. read section 5). D-O by passed the problem of finding the \( U(x) \) by solving the B-D system of PDE’s. They simply guessed correctly the potential.

**Remark F.4.** Eq.(F.3) is exactly of the same type as Eq.s(3.14),(3.35). Therefore, methods described in section 3, also involving solutions of PDE’s should be considered as complementary to those in [70],[144],[145].

**Remark F.5.** There are three types of Laplace-type conformally superintegrable equations. These are:

a) Recasting a Helmholtz superintegrable system \( H \Psi = E \Psi \) into the Laplace-type form \( H' \Psi = 0, H' = H - E \). Here \( E \) is absorbed into potential as a parameter. Clearly, this is the case of Sturmian Eq.(F1.b).

b) Replacing a Helmholtz superintegrable system \( H \Psi = E \Psi \) by the Laplace-type \( H' \Psi = 0 \) in which \( H' = H - E_0 \) with \( E_0 \) fixed once and for all eigenvalue. This is again the Sturmian-type problem.
c) Begin with a Helmholtz-type equation \( H \Psi = E \Psi \) which is not superintegrable and convert it into a Laplace-type. The resulting equation will have the induced conformal symmetries.

**Remark F.6.** Just described classification justifies the transition from Eq.(1.2) to Eq.(1.3).

**Appendix G. Thomas-Fermi treatment of multielectron atoms.**

**Contributions of Fermi, Tietz and Klechkowski into proof of the Madelung rule**

Although the Thomas-Fermi (T-F) method is only asymptotical (works well in the limit of high electron densities), because of its simplicity and reasonably good accuracy, we provide some information about this method which is helpful for extension of the formalism of the main text to multielectron atoms cases. The T-F method and contributions by Tietz to this method used in section 4.5 are concisely summarized in the book by Flugge [24]. Belokolos [40] used the Tietz potential (Eq.s(G.8),(G.9)) for the WKB-assisted "proof" of the Madelung rule. His results are neither exact not conclusive even though he is citing the paper by Wong [123] in which the Madelung rule is seemingly derived. In his derivation Wong used the Tietz potential. Wong’s results are solely based on works by Fermi [125], Tietz [24] and Klechkowski [146]. It is impossible to develop theory of the Madelung rule without acknowledging contributions of these authors. The strongest and chronologically the earliest contribution to this topic was made by Fermi. Following publication of his ground breaking paper on the T-F method in 1927, in 1928 Fermi came up with the paper [125] describing applications of the T-F method to the periodic system of elements. In it he posed and solved the following problem: find analytically a relationship between the atomic number \( Z \) and the number of electrons \( N_l \) with azimuthal number \( l \). Knowledge of such a relationship allows then to solve the related problem of major significance: find a sequence of \( Z \)'s for which for the first time electrons with azimuthal numbers \( s, p, d, f, \ldots \) emerge. Fermi found the sequence : 1, 5, 21, 58. These are exactly the atomic numbers initiating sequential irregularities in filing of the periodic system. Subsequently, Tietz [147], [148] simplified Fermi calculations with help of the potential bearing his name. The whole book by Klechkowski on proving the Madelung rule is effectively a discussion around these two works by Tietz [147], [148]. The paper by Wong is a condensed summary of the results by Klechkowski summarized in his book [147]. As such, it suffers from the same drawbacks as Klechkowski’s book. Specifically, in his book Klechkowski discusses from various perspectives the result by Tietz for \( N_l \):

\[
N_l = 2(2l + 1)(6Z)^{\frac{1}{3}} - 2(2l + 1)^2.
\]  

Eq.(G.1) coincides with Eq.(14) of Wong’s paper [123] where it was derived independently based directly on ideas by Fermi. Next, following Klechkowski’s philosophy, Wong runs into myriad of the same kinds of problems. They begin from an assumption

\[
\frac{N_l}{2(2l + 1)} \simeq n - l - 1 = n_r.
\]  

\[\text{(G.2)}\]
Here \( n \) and \( n_r \) are respectively the principal and radial quantum numbers. A comparison between Eq.s (G.1) and (G.2) then produces:

\[
(6Z)^{\frac{1}{3}} - (2l + 1) = n - l - 1. \tag{G.3a}
\]

However, already from Eq.(G.1) it is evident that on the l.h.s the \( N_l \) should be a nonnegative integer while on the r.h.s. the term \((6Z)^{\frac{1}{3}}\) is making the r.h.s. noninteger for general \( Z' \)'s. Since Eq.(3.Ga) is incorrect for arbitrary nonnegative \( Z' \)'s, the same is true for its corollary

\[
n + l = (6Z)^{\frac{1}{3}}. \tag{G.3b}
\]

Wong claims, however, that this result is mathematically equivalent to the Madelung rule. Since \((6Z)^{\frac{1}{3}}\) is not always an integer, the rest of Klechkowski's book [146] is devoted to finding some corrections to Eq.(G.1) making \( n + l \) an integer. Wong missed this issue (studied by Klechkowski) completely. His paper entitled "Theoretical justification of the Madelung rule" culminates in Eq.(G.3b). None of the corrections discussed in Klechkowski book are rigorous, systematic or convincing. Surprisingly, he made no attempts to use directly the results of Fermi. Instead, he made a few comments on the paper by Ivanenko and Larin [124] which, in our opinion, deserves more attention than that given to it by Klechkowski. The authors of [124] used the Thomas-Fermi-Dirac method to recalculate the results by Fermi in a direct and simple way. The final result is expressible in compact form:

\[
Z_l = \frac{\gamma(Z_l)(2l + 1)^3}{(2l + 1)} \tag{G.4}
\]

The \( Z_l \)-dependent factor \( \gamma(Z_l) \) is calculated iteratively for each \( Z_l \). Fig.1 of [124] indicates that this variable factor can be safely replaced by the constant factor: \( \gamma(Z_l) \simeq 0.169 \). In such a case use of Eq.(G.4) reproduces (by rounding the numbers in Eq.(G.4)) the Fermi sequence of \( Z' \)'s: 1 \((l = 0)\), 5 \((l = 1)\), 21 \((l = 2)\) and 58 \((l = 3)\).\(^{49}\) Strictly speaking, the minimization procedure involved in obtaining Eq.(G.4) is not extendable to the values of \( Z \) significantly different from those in the Fermi sequence. In his book Klechkowski missed this restriction completely. If however, in Klechkowski style, we do use Eq.(G.4) with unrestricted \( Z' \)'s in Eq.(G.3b) in order to obtain

\[
n + l = (6Z)^{\frac{1}{3}} = (6 \cdot 0.169)^{\frac{1}{3}}(2l + 1) = 1.004645(2l + 1) \simeq 2l + 1 \tag{G.5}
\]

then, since \( n = n_r + 1 + 1 \), Eq.(G.5) reduces to the identity, if \( n_r = 0 \). This requirement makes some physical sense as explained in section 5.

Now we are in a position to make a number of comments about the Tietz potential. In the book by Flugge [24] in sections devoted to the T-F theory our readers will find a nice discussion about the Tietz potential and how it fits the T-F theory. Typically, readers with standard physics background are left with an impression that the T-F theory is reasonably well describing multielectron atoms only when the number of electrons tend to infinity and is

\(^{49}\) Evidently, Fermi also used some rounding.
useless for description of, say, a hydrogen or helium atom. In the lecture notes by Roi Baer [149] it is demonstrated that, surprisingly, the T-F theory provides reasonable results even for a hydrogen atom. Additional details on T-F theory (without uses of the Tietz potential) are beautifully summarized in the book by March [27].

To develop our intuition at this stage of our presentation the scaling analysis by Feynman, Metropolis and Teller [150] is the most helpful. Following these authors, we consider a similarity transformations for an atom. They are consisting of increasing the nuclear charge of an atom while simultaneously increasing the number of electrons so that the atom remains neutral. Evidently, such a transformation is describing a relation between solutions for various nuclear charges. It is assumed that the De Broglie length \( \lambda \) remains unchanged under scaling. Transformations consists of the following infinitesimal changes:

\[
Z \rightarrow Z(1 + \zeta), \quad r \rightarrow r(1 + \rho), \quad \bar{E} \rightarrow \bar{E}(1 + \eta).
\]

Here \( \bar{E} \) represents any form of the energy (classical or quantum) per electron. At the same time, the electron density \( q \) is changed by \( q(1 + \nu) \).

Elementary calculation based on these results produces:

\[
\rho = -\frac{1}{3}\zeta \quad \text{and} \quad \eta = \frac{4}{3}\zeta.
\]

Thus, the energy \( \bar{E} \) per electron changes as \( \bar{E}(1 + \frac{4}{3}\zeta) \) and for neutral atom initially made of \( Z \) electrons it changes as \( \bar{E}(1 + \frac{4}{3}\zeta)Z(1 + \zeta) = \bar{E}Z(1 + \frac{7}{3}\zeta) \). Since in these arguments we assumed the validity of T-F relationship \( \bar{E} = \kappa q^2 \), the dimensionless T-F equation

\[
\frac{d^2\varphi}{dx^2} = \frac{\varphi^3}{\sqrt{x}}
\]

connected with this relationship automatically establishes the characteristic length scale parameter

\[
a = 0.8853 a_0 Z^{-\frac{1}{4}},
\]

where \( a_0 \) is the Bohr radius, \( a_0 = \frac{\hbar^2}{me^2} \). From here emerges the dimensionless length scale: \( x = \frac{r}{a} \). As before, we shall use the system of units in which \( \hbar = m = 1 \). In view of just presented results, the potential energy of electron scales as \( Z/a \simeq Z^{\frac{4}{3}} \) so that for \( Z \) atomic electrons the total energy scales as \( Z^{\frac{7}{3}} \). This result is consistent with previously obtained scaling result \( \bar{E}Z(1 + \frac{4}{3}\zeta) \) for the total energy. The result \( Z^{\frac{7}{3}} \) was first derived by Milne [27]. Schwinger [151] obtained a correction to just obtained scaling result. With it, such a correction gives good results for all \( Z \)'s. This fact, is of importance if one is interested in comparing much more technically cumbersome Hartree-Fock and T-F theories. Another example of this kind is related to discussion related to the Tietz potential. The origins of this potential are connected with study of solutions of T-F Eq. (G.6). This nonlinear equation does not admit exact analytical solution and, in addition, it requires the assignment of boundary conditions. For neutral atoms these are simple: \( \varphi(0) = 1 \) and \( \varphi(\infty) = 0 \). Because of their
simplicity, Tietz suggested the analytical form for $\varphi$:

$$\varphi(x) = \frac{1}{(1 + \alpha x)^2}, \quad \alpha = 0.53625.$$  \hspace{1cm} (G.8)

The constant $\alpha$ is not a fitting parameter. It is determined by the electroneutrality normalization condition [24]. The Tietz potential $V(x)$ is obtained with help of $\varphi(x)$ as follows

$$V(r) = -\frac{Ze}{r} \varphi \left( \frac{r}{a} \right)$$  \hspace{1cm} (G.9)

For $r \to 0$, $V(r)$ tend to the usual attractive Coulombic potential while for larger $r$'s it represents $V_{\text{eff}}(r)$ introduced in Eq.(1.2). This fact was reported in [25] on p.664, Fig.10. From this figure it follows that the plot of $\varphi(x)$ vs. $x$ obtained with help of the T-F method practically coincides with that obtained numerically with help of the Hartree-Fock method.

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