A new discrete view to quantum mechanics

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Abstract

Here I present a new discrete model of quantum mechanics for relativistic 1-electron systems, in which particle movement is described by a directed space-time graph with attached 4-spinors, but without any continuous wave functions. These graphs only consist of few space-like edges, e.g. the ground state of atoms is described by two nodes and one edge, and interactions only take place at the nodes.

The fundament is an extremal principle for a relativistic invariant "LAGRANGian sum", from which "field-equations" and "equations of motion" are derived, so the states (including the graph nodes) are completely determined.

As important validations of the model, the corresponding graphs for the stationary DIRAC-equation for the atom are drawn and the correct spectra are computed (SOMMERFELD-levels).

Also a discrete SCHRÖDINGER approximation and an associated "HAMILTONian sum" are derived and the correct equation of a classical moving particle under LORENTZ-force is presented.

I hope, that this new approach will help, to overcome some problems of current quantum mechanics by making the wave function superfluous.

Contents

1 Introduction

In this paper, I propose a new discrete view to the quantum world, without the use of a wave function concept.

The wave function was introduced by ERWIN SCHRÖDINGER around 1925 to describe quantum mechanical states, like electrons inside an atom, for which classical descriptions failed.

However, there is a long, unceasing discussion about the interpretation of this wave function, especially for the measurement process ("collapse" of wave function) (see e.g. [10] or [1] pp. 40, for a comprehensive discussion).
On the other hand, it seems paradox, that the description of discrete quantum states (like energy levels of an atom) required the invention of a new continuous field. This new field has the additional strangeness, to be 'not physical', i.e. is not directly measurable, like all other known fields.

Additionally, the current QED-theory has severe difficulties arising from infinite integrals, which have to be eliminated by some mathematical tricks (renormalization). Many physicists believe, that these are at least suspicious (see e.g. [8], p. 458, [2], pp. 166). As far as I see, the theory presented here, will not show any infinite values.

As strong motivation to try discrete theories, I want to cite A. EINSTEIN from one of his last works (see [5], Appendix II, 1954, p. 163): "Man kann gute Argumente dafür anführen, daß die Realität überhaupt nicht durch ein kontinuierliches Feld dargestellt werden könne. Aus den Quantenphänomenen scheint nämlich hervorzugehen, daß ein endliches System von endlicher Energie durch eine *endliche* Zahl von Zahlen (Quanten-Zahlen) *vollständig* beschrieben werden kann. Dies scheint zu einer Kontinuums-Theorie nicht zu passen und muß zu einem Versuch führen, die Realität durch eine rein algebraische Theorie zu beschreiben. Niemand sieht aber, wie die Basis einer solchen Theorie gewonnen werden könnte."[1] [2]

Nowadays, there exist several proposals to introduce 'discreteness' into physics. Most of them postulate a space-time lattice at the PLANCK-scale, of about $10^{-33}cm$ and $10^{-44}s$. These scales are assumed to play a fundamental role in general relativistic quantum gravitation (which is not considered in this article). However, due to the smallness of these units, it is not to expect to find consequences of the lattice structure with currently available measurement techniques. The quantum fields in these theories mostly appear as continuous approximations of discrete lattice fields.

My approach is different to the above mentioned, since it considers discreteness at particle wavelength scales ($\sim 1/m$ for time-like edges, COMPTON-wavelength),[3] i.e. much larger, so it is directly related to the quantum nature of the particle.
On the other hand, I do not describe the whole space-time as a gridded structure, only the movement of the elementary particles should be considered as not being continuous but in finite steps. There might exist an underlying PLANCK-scale grid, but this is not needed in the following considerations.

In this paper, I deal with a new view to special relativistic quantum mechanics of spin-1/2 particles in electromagnetic fields, i.e. DIRAC equation and their solutions (in flat MINKOWSKI space-time), where the wave function is a 4-dimensional complex field.

[1] Emphasations by A. Einstein

[2] Translation: "There are good arguments, that reality cannot be represented by a continuous field. It seems to follow from quantum phenomena, that a finite system of finite energy can be described *completely* by a *finite* number of numbers (quantum numbers). This seems not to fit to a continuum-theory and must lead to the attempt to describe reality by a pure algebraic theory. Nobody sees, however, how the basis for such a theory can be achieved.

[3] In this article I use "natural units", where $\hbar = 1$ and $c = 1$ holds.

In the discrete theory proposed here, the moving particle[4] is described as a set of space-time points, with finite space extent and, of course, infinite time extent. Attached to each time-like edge is a DIRAC-spinor (as a constant) which replaces the continuous spinor field.

It turns out, that the number of points required to model e.g. the energy levels of the atom, is only in the order of the quantum numbers. In this (stationary) case the time-edges of the graph are simply equal and the space edges are constant. In nonstationary cases, however, also graphs with bifurcations and combinations are imaginable, but these are not considered in this article.

The equations for both grid-points and spinors are derived from an extremal principle of *one general sum-function*. This seems to be the most appealing aspect of this new theory. All other discrete theories, known to me, postulate some preset, fixed grids, which are not influenced by the fields.[5]
This extremal principle resembles a LAGRANGE functional, which is widely used in quantum physics and esp. quantum field theory. Here, the LAGRANGian is replaced, of course, by a sum over the space-time graph and the variational principle simply maps to the variations of the points and spinors.

To show the correctness of the theory two important cases are discussed and computed below: the stationary electron in the COULOMB-field (atom) and an electromagnetic acting particle in nonstationary case (accelerated by LORENTZ-force).[6]

A last word to the *structure* of this article. Some of the evaluations are not strictly needed in this paper, esp. the simple start cases. However, it is to expect, that many readers are not very familiar with the unusual notations used here. Thus, I think it is always better to start with the simplest possible cases and then proceed to the more complex states.

In any case, I tried to put the evaluations straightforwardly as possible. So many proofs are left out, or shifted to the numerous footnotes, so that quick readers can skip them. Longer ones were put into the appendix, which thus became quite voluminous. It also serves, to illustrate the correspondencies to classical theories and formalisms.

[4] Of course, resting particles can be described as special stationary cases.

[5] In some vague sense, this resembles the concept of general relativity, where the space-time metric $g_{\mu\nu}$ is influenced by the mass distribution.

[6] Since most formulas derived there, are simple algebraic, they can easily be implemented in numerical computer programs. In fact, I have done this for most of the examples, to validate the evaluations numerically.

2 Notations, Entities and Transformations

In contrast to the usual description of DIRAC-spinors as 4-spinors, I use a slightly different notation by 'spinor-matrices'. These are complex 2x2-matrices, i.e. they have the same number of components.[7]
MINKOWSKI-vectors and LORENTZ-transformations are then represented as certain *subsets* of these 2x2-matrices, with constraints explained below.

In the appendix it is shown, that both notations are equivalent for the DIRAC-equation and classical relativistic electromagnetism.

The main reason for using this form is, that *all entities* are represented by the *same algebraic structure*, and many of the following equations are much better readable, than in component notation.

General 2x2-matrices are here denoted with uppercase letters $P, Q, S, \ldots$.
The usual operations with the matrix $P = \binom{a,b}{c,d}$, with complex a, b, c, d, here are written as:[8]

- $\bar{P} = \binom{d,-b}{-c,\ a}$: adjuncted matrix of P,[9]
- $|P| = ad - bc$: the scalar determinant, with $P\bar{P} = I\,|P|$,
- $\mathcal{T}(P) = a + d$: the scalar trace, with $P + \bar{P} = I\,\mathcal{T}(P)$,
- $P^T = \binom{a,c}{b,d}$: the transposed, $P^* = \binom{a^*,b^*}{c^*,d^*}$ the complex conjugated,
- $P^\dagger = (P^*)^T = \binom{a^*,c^*}{b^*,d^*}$: the adjungated (or HERMITEan conjugated).[10]

Since it is often needed in the following, and not quite obvious, I state here the general circularity relation for the trace of any matrices $ABC, \ldots, X$: $\mathcal{T}(A\,BC \ldots X) = \mathcal{T}(BC \ldots X\ A)$.[11]

A MINKOWSKI-*vector* is in this formalism represented by a HERMITEan matrix, and here denoted by boldface (upper- and lowercase) letters:[12] $\mathbf{M}^\dagger = \mathbf{M}$, to distinguish it from other matrices (spinors, transformations, electromagnetic field tensor).
It has, of course, 4 real components, which can be mapped to space-time coor-

[7] They may be thought of writing the two bi-spinors as a two-column matrix, see Appendix.
[8] I denotes the 2x2-identity matrix.
[9] The inverse matrix of P is then, of course $P^{-1} = \bar{P}/|P|$.
[10] All operations here commute, e.g. $\overline{(P^\dagger)} = (\bar{P})^\dagger$ and products obey $(PQ)^\dagger = Q^\dagger P^\dagger$ and $\overline{(PQ)} = \bar{Q}\bar{P}$.
[11] It can be derived from the symmetry relation $\mathcal{T}(AB) = \mathcal{T}(BA)$, which again follows e.g. from $|A + \bar{B}| = (A + \bar{B})(\bar{A} + B) = |A| + |B| + \mathcal{T}(AB) = |B + \bar{A}|$.
[12] One exception is the relativistic ∂-operator.

dinates (t, x, y, z) in the following way (see e.g. [9], pp. 16):[13]

$$\mathbf{M} = \begin{pmatrix} t+z, x-iy \\ x+iy, t-z \end{pmatrix} = tI + x\sigma_1 + y\sigma_2 + z\sigma_3, \tag{1}$$

where σ_i are the usual PAULI-matrices.

LORENTZ-*transformations* are represented by unimodular matrices $T, |T| = 1$, and thus have 6 real degrees of freedom.[14] Ordinary space rotations additionally fulfill the condition $T^\dagger = \overline{T}$, leaving 3 free real degrees,[15] while special LORENTZ-transformations obey $T^\dagger = T$.[16]

With respect to their behaviour under space-time transformations, we must distinguish between spinor- and MINKOWSKI-matrices.

Let T be a LORENTZ-transformation, then a spinor transforms with $P \to TP$ (then follows e.g. $P^\dagger \to P^\dagger T^\dagger$), while a MINKOWSKI matrix transforms with $\mathbf{M} \to T\mathbf{M}T^\dagger$.[17]

The determinant $|\mathbf{M}|$ is then obviously the MINKOWKSKIan *invariant*[18] (always real):

$$|\mathbf{M}| = t^2 - x^2 - y^2 - z^2. \tag{2}$$

It is remarkable in this formula, that the signature of the metric tensor $(+---)$ automatically follows from the property of HERMITEcity.

To build the general *scalar product* of two MINKOWSKI matrices $\mathbf{A}, \mathbf{B}$ serves the formula, which is obviously also invariant and real:

$$\mathcal{T}(\mathbf{A}\bar{\mathbf{B}}) = \mathcal{T}(\mathbf{B}\bar{\mathbf{A}}). \tag{3}$$

From the representation (1) should also be noted, that the trace of a MINKOWSKI matrix maps to the *time component*, and the operation of "adjunction" is a space (R^3) inversion.

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[13] Since every matrix M can be uniquely decomposed into a HERMITEan and anti-HERMITEan part by $M = \mathbf{A} + i\mathbf{B}$, with $\mathbf{A}^\dagger = \mathbf{A}$, $\mathbf{B}^\dagger = \mathbf{B}$ (which then transform independently under LORENTZ-transformations), all 2x2 matrices can be seen as generalization of MINKOWSKI-matrices.

[14] Mathematically speaking, in terms of LIE-group theory, T build the $SL(2, \mathcal{C})$-group, which is a double cover of the LORENTZ-group.

[15] By this definition they build a subgroup (the *quaternion group*, see appendix), while special LORENTZ-transformations do not.

[16] E.g. a matrix $T = \left(\begin{smallmatrix} \beta, 0 \\ 0, 1/\beta \end{smallmatrix}\right)$ with real β, performs a (t, z) transformation.

[17] The above condition for space rotations $T^\dagger = \overline{T} = T^{-1}$ then leads to $\mathbf{M} \to T\mathbf{M}T^{-1}$, consequently the trace of $\mathcal{T}(\mathbf{M}) = 2t$ is invariant, as required.

Consider e.g. the transformation $T = i\sigma_1$, which performs a rotation of 180° around the x-axis. A full rotation is then represented by $T = (i\sigma_1)^2 = -1$.

[18] The proof of invariance is simple: $|\mathbf{M}| \to |T||\mathbf{M}||T^\dagger| = |\mathbf{M}|$, since $|T| = 1$

3 Space-Time Graph and "LAGRANGE-Sum"

3.1 Descriptions of Particle Movement in SRT

This short section is intended to explain concisely, how particle movement is described in the context of *Special Relativity* and MINKOWSKI space-time. Also a discrete variant of movement (which is not used in the following) is sketched, but quantum effects are not considered here.

A *continuous relativistic particle trajectory* is given by a space-time curve i.e. the 4 functions $\mathbf{x}(\tau) = (x(\tau), y(\tau), z(\tau), t(\tau))$[19] which is usually parametrized by the *eigentime* τ.[20]
This τ is defined by $d\tau^2 = |d\mathbf{x}| = dt^2 - dx^2 - dy^2 - dz^2$.

Since $d\tau^2$ is an invariant, all MINKOWSKI-vectors $d\mathbf{x}$ can be classified by its sign: $d\tau^2 > 0$: time-like, $d\tau^2 = 0$: light-like, $d\tau^2 < 0$: space-like.

Usually by the condition of causality it is required, that no interactions over space-like separated regions occur. The movement of a particle is restricted to time-like vectors (resp. light-like for massless particles).

The *discrete* form of such a space-time curve is then simply a sequence

$$\mathbf{x}_1 = (x_1, y_1, z_1, t_1), \quad \mathbf{x}_2 = (x_2, y_2, z_2, t_2), \quad \dots$$

This sequence can be considered as a graph with the edges $(\mathbf{x}_k \to \mathbf{x}_{k+1})$, which describe a movement in finite "jumps" and "time-likeness" here obviously means $|\mathbf{x}_{k+1} - \mathbf{x}_k| > 0$.

The (continuous) movement of a classical charged particle in an electromagnetic field (LORENTZ-force) can also be derived from a variation principle for a LAGRANGian .

Let all possible space-time curves be parametrized by a parameter $\lambda : \mathbf{x}(\lambda)$. In matrix notation the action integral is then written:[21]

$$\mathcal{L}(\mathbf{x}(\lambda)) = \int_{\lambda_1}^{\lambda_2} d\lambda \left[m \left|\left| \frac{d\mathbf{x}}{d\lambda} \right|\right| + e\mathcal{T}(\bar{\mathbf{A}}(\mathbf{x}) \frac{d\mathbf{x}}{d\lambda}) \right].$$

The variation of space-time curve $\mathbf{x}(\lambda) = \mathbf{x}_e(\lambda) + \delta\mathbf{x}(\lambda)$ results in an extremal curve $\mathbf{x}_e(\lambda)$.
Then λ is identified with the eigentime of the extremal curve $d\tau \stackrel{def}{=} ||d\mathbf{x}_e||$.

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[19] Or in matrix notation written as: $\mathbf{x}(\tau) = \begin{pmatrix} t(\tau)+z(\tau), x(\tau)-iy(\tau) \\ x(\tau)+iy(\tau), t(\tau)-z(\tau) \end{pmatrix}$.

[20] But also other parameters, e.g. t may be used. The advantage of using τ is, that the velocity vector $\mathbf{u} = \frac{d\mathbf{x}}{d\tau}$ is then normalized to unity.

[21] absolute value of a MINKOWSKI vector written as $||\mathbf{x}|| \stackrel{def}{=} \sqrt{|\mathbf{x}|}$

The extremal curve is then given by the equation of LORENTZ-force:[22]

$$m\frac{d^2\mathbf{x}}{d\tau^2} = \frac{e}{2}\left(\frac{d\mathbf{x}}{d\tau}F + F^\dagger\frac{d\mathbf{x}}{d\tau}\right).$$

It is interesting to state here, that there exists also *discrete representations* of the above LAGRANGian formalism. However, this example is given as illustration only, and *not used in the following sections!*

A possible *discrete* variant of the above integral is:

$$\mathcal{L} = m\sum_k ||\mathbf{x}_{k+1} - \mathbf{x}_k|| + e\sum_k \mathcal{T}(\bar{\mathbf{A}}(\mathbf{x}_k)(\mathbf{x}_{k+1} - \mathbf{x}_{k-1})).$$

Herein the variation of one space-time point (node) $\mathbf{x}_k$ leads to a *discrete* version of the LORENTZ-Force:

$$m\left(\frac{\mathbf{x}_{k+1} - \mathbf{x}_k}{||\mathbf{x}_{k+1} - \mathbf{x}_k||} - \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{||\mathbf{x}_k - \mathbf{x}_{k-1}||}\right) \approx \frac{e}{2}\left((\mathbf{x}_{k+1} - \mathbf{x}_{k-1})F_k + F_k^\dagger(\mathbf{x}_{k+1} - \mathbf{x}_{k-1})\right).$$

Like in the following sections, here also the identifaction $||\mathbf{x}_{k+1} - \mathbf{x}_k|| = 1/m$ is possible, since this expression is conserved (approximately).[23]

3.2 General Considerations with Space-Time Graphs

Space-time grids are commonly used to solve partial differential equations, e.g. numerically. Then integrals (e.g. the LAGRANGian functional) are represented as sums. Usually, the gridded structure is viewed as approximation of the continuum, and the smaller the edges are, the better the approximation.
In this theory, I try another point of view: the grid represents the quantum state and the differential form is the approximation.
In fact, it turns out in the following, that e.g. to describe bound states in the atom, that there exist "minimal grids", which suffice to represent the *exact states* in the DIRAC-theory.
It should be noted, however, that the usage of *finite* (esp. space-like) edges introduces some kind of nonlocality and causality violation into the theory.[24]

I will start with the general expression for the "LAGRANGian sum" over any graph. Let $\{\mathbf{x}_i\}$ be the nodes as MINKOWSKI matrices (numbered in an arbitrary order), $\mathbf{H}_{ij}, \mathbf{M}_j$ be some MINKOWSKIan matrices, $\mathbf{A}$ the electromagnetic vector potential, which has the values $\mathbf{A}_i \stackrel{def}{=} \mathbf{A}(\mathbf{x}_i)$ at the grid points, and P_i some spinors:[25]

[22] See Appendix for the relations between $\mathbf{A}$ and F in matrix notation.

[23] This has no analogon in the continuous case. To prove it, multiply the eq. with $\bar{\mathbf{q}} \stackrel{def}{=} \bar{\mathbf{x}}_{k+1} - \bar{\mathbf{x}}_{k-1}$ (e.g. from left) and take the trace (i.e. building scalar product with $\mathbf{q}$), Then the r.h.s. vanishes, since $\mathcal{T}(F) = \mathcal{T}(F^\dagger) = 0$.

[24] Also should be added, that the used graphs show some similarities to FEYNMAN-graphs. However, bifurcations are not considered here, and the mathematical background is completely different.

[25] As usual, m denoting particle mass, e electrical charge and $\Re()$ the real part of a complex number.

$$\mathcal{L} = \sum_{ij} \mathcal{T}((\mathbf{x}_i - \mathbf{x}_j)^{-1}\mathbf{H}_{ij}) + e\sum_i \mathcal{T}(\bar{\mathbf{A}}_i\mathbf{M}_i) - 2m\sum_i \Re(|P_i|). \qquad (4)$$

However, the first double sum is not to be applied for all pairs (i, j), but only for edges.
The auxiliary matrices $\mathbf{H}_{ij}, \mathbf{M}_i$ in this equation shall be constructed as HERMITEan bilinear forms from the fundamental spinors P_i, as explained below.

At first, however, it is to prove, that this sum fulfills all requirements for a "LAGRANGian": it is a real scalar and invariant under all LORENTZ transformations.

It is obviously scalar, by construction. To prove the reality of $\mathcal{L}$, I state that:

- for any HERMITEan matrix $\mathbf{A}$ holds trivially: $\mathcal{T}(\mathbf{A}) = real$,
- for any two HERMITEan matrices $\mathbf{A}, \mathbf{B}$ holds: $\mathcal{T}(\mathbf{AB}) = real$, due to the symmetry relations: $\mathcal{T}(\mathbf{AB}) = \mathcal{T}(\mathbf{BA}) = \mathcal{T}(\mathbf{B}^\dagger\mathbf{A}^\dagger) = \mathcal{T}((\mathbf{AB})^\dagger)$.

Since all factors are HERMITEan matrices and $\Re(|P|)$ is always real, the complete sum is real.

To prove LORENTZ invariance, I state, that the epressions $\mathbf{x}^{-1}$ and $\bar{\mathbf{A}}$ transform with $\bar{T}^\dagger(\cdot)\bar{T}$ and therefore the expressions $\mathcal{T}(\mathbf{x}^{-1}\mathbf{H})$ and $\mathcal{T}(\bar{\mathbf{A}}\mathbf{M})$ are invariant scalar products.
The determinant $|P|$ is trivially invariant under LORENTZ-transformations, if the spinor transformation rule $P \to TP$ is considered, q.e.d.

3.3 Regular Space-Time Graphs

Now I consider *regular* space-time graphs. The restriction to these graphs is mainly due to the problem, that it is not yet clear, what physical conditions can lead to bifurcations or combinations, and the mathematical difficulties in handling them.
This is no principal limitation, and as shown in the following, many problems of one-particle quantum mechanics can be described with these graphs.

One first introduces double indices for the nodes $\{\mathbf{x}_{ik}\}$, where the first index should stand for space, while the second index k stands for time steps (thus unbounded, $k = -\infty \cdots \infty$).[26]

The regularity condition then means, for any time index k there exist n nodes: $i = 1, \ldots, n$ and that for any i, j, k should hold $|\mathbf{x}_{ik} - \mathbf{x}_{jk}| < 0$ (space-like edge), and for any i, k: $|\mathbf{x}_{i,k+1} - \mathbf{x}_{i,k}| > 0$ (time-like edge) and also $t_{i,k+1} - t_{i,k} = \frac{1}{2}\mathcal{T}(\mathbf{x}_{i,k+1} - \mathbf{x}_{i,k}) > 0$ (direction of time arrow). Also, only

[26] This numbering scheme does not violate the LORENTZ-covariance of the following evaluations.

timely consecutive nodes $(k, k+1)$ shall be connected by an edge.

The (constant) spinors P_i are now considered to be assigned uniquely to the *time-like edges* (not to the nodes): $(\mathbf{x}_{i,k+1}, \mathbf{x}_{i,k}) \leftrightarrow P_{ik}$.
Of course, this assumption introduces a fundamental asymmetry between space and time and leads to different formulas for the above introduced $\mathbf{H}$.
For space-symmetry reasons, the following ansatz is suggested:
$\mathbf{H}_{i,k+1,i,k} = P_{ik}P_{ik}^\dagger$, $\mathbf{H}_{i,k,j,k} = P_{i,k-1} \circ P_{j,k}$,[27] (all other combinations of indices have no edge assigned) and $\mathbf{M}_{ik} = \frac{1}{2}(P_{ik}P_{ik}^\dagger + P_{ik-1}P_{ik-1}^\dagger)$.[28]
Then from (4) results:

$$\begin{aligned}\mathcal{L} &= \sum_{k,i} \mathcal{T}((\mathbf{x}_{i,k+1} - \mathbf{x}_{i,k})^{-1} P_{ik}P_{ik}^\dagger) \\ &+ \sum_{k,ij} \mathcal{T}((\mathbf{x}_{i,k} - \mathbf{x}_{j,k})^{-1} \frac{1}{2}(P_{i,k-1}P_{j,k}^\dagger + P_{j,k}P_{i,k-1}^\dagger)) \\ &+ e\sum_{k,i} \mathcal{T}(\frac{1}{2}(\bar{\mathbf{A}}_{\mathbf{i},\mathbf{k+1}} + \bar{\mathbf{A}}_{\mathbf{i},\mathbf{k}})P_{ik}P_{ik}^\dagger) - 2m\sum_{ik} \Re(|P_{ik}|).\end{aligned} \tag{5}$$

To visualize the kinematic terms (first and second term) of this sum, the following picture is used, where the spatial extent number is set to $n = 2$ (this example graph e.g. also represents the ground state of an electron in an atom):

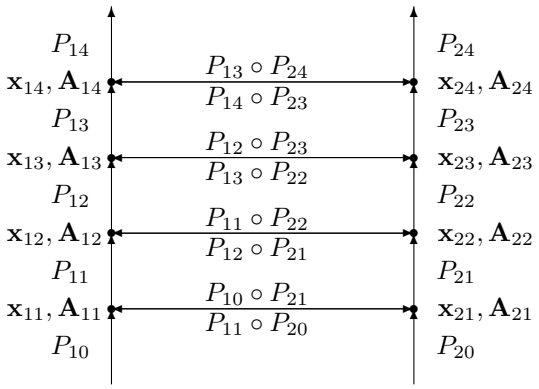

Fig. 1: example space time graph (time axis vertical)

The *extremal principle* now considers the sum $\mathcal{L}$ as a function of all inner variables $\mathbf{x}_{ik}, P_{ik}$, whereas possibly some boundary variables have to be fixed, to account for initial conditions:

$$\mathcal{L}(\mathbf{x}_{ik}, P_{ik}) \to Extr. \tag{6}$$

[27] The circle stands for the HERMITEan conjugated expression: $P \circ Q \stackrel{def}{=} \frac{1}{2}(PQ^\dagger + QP^\dagger)$.
[28] all obviously HERMITEan

3.4 Simplest Case

To demonstrate the method of deriving the "field equations" and "equations of motion" from this principle, I start with the simplest case: no electromagnetic potential ($\mathbf{A} = 0$) and the graph has only one spatial index: $n = 1$.
This model represents a freely moving spin-1/2 particle.

The graph then reduces to a sequence of MINKOWSKI space-time points, which is actually a discrete particle trajectory, as explained in the section 3.1.

The spatial index can be omitted, and the second and third sum in equation (5) are zero. It remains the sum:

$$\mathcal{L}(\mathbf{x}_k, P_k) = \sum_k \mathcal{T}((\mathbf{x}_{k+1} - \mathbf{x}_k)^{-1} P_k P_k^\dagger) - 2m \sum_k \Re(|P_k|). \tag{7}$$

This sum is obviously invariant under the "local" transformations $P_k \to P_k S_k$, when $S_k S_k^\dagger = |S_k| = 1$.[29] That means, the spinors P_k are determined only up to these factors by the following equations (gauge invariance).

At first, I consider the variation of one specific P_k, in this sum. This variation is similar to the usual methods in quantum theories.
For the variation of the real part of the determinant, is used: $2\Re(|P|) = |P| + |P^\dagger|$ and

$$|P + \delta P| = (P + \delta P)(\overline{P + \delta P}) \approx |P| + \delta P \overline{P} + P \overline{\delta P} = |P| + \mathcal{T}(\delta P \overline{P}), \tag{8}$$

therefore results from substitution $P_k \to P_k + \delta P_k$ the variation

$$\delta\mathcal{L} = \mathcal{T}((\mathbf{x}_{k+1} - \mathbf{x}_k)^{-1}(\delta P_k P_k^\dagger + P_k \delta P_k^\dagger) - m\mathcal{T}(\delta P_k \overline{P}_k + \delta P_k^\dagger \overline{\delta P_k^\dagger}). \tag{9}$$

To simplify the formulas, I define an auxiliary variable $\mathbf{v}_k \overset{def}{=} (\mathbf{x}_{k+1} - \mathbf{x}_k)^{-1}$, so equation (9) writes (after using the general circularity relations for the trace):

$$\delta\mathcal{L} = \mathcal{T}(\delta P_k (P_k^\dagger \mathbf{v}_k - m\overline{P}_k)) + \mathcal{T}(\delta P_k^\dagger (\mathbf{v}_k P_k - m\overline{P_k^\dagger})). \tag{10}$$

As usual, the variations of δP_k and $\delta P_k^\dagger$ are considered as independent, therefore both terms must vanish. An expression $\mathcal{T}(XY)$, however, can only vanish for any matrix X, if $Y = 0$ holds. So the two (equivalent, since by definition $\mathbf{v} = \mathbf{v}^\dagger$) equations result:

$$P_k^\dagger \mathbf{v}_k = m\overline{P}_k \quad \text{and} \quad \mathbf{v}_k P_k = m\overline{P_k^\dagger}. \tag{11}$$

This equation corresponds to the usual "field equations" in quantum mechanics. Here it forces (by taking the determinant on both sides) that, since $|\mathbf{v}_k| = real$, also $|P_k| = |P_k^\dagger| = real$, consequently $|\mathbf{v}_k| = m^2 = const.$ or $|\mathbf{x}_{k+1} - \mathbf{x}_k| = 1/m^2$, implying that the motion vector is a time-like vector of the constant length $1/m$.[30]

[29] These S are normalized *quaternions*, see appendix.

[30] In the rest frame of the particle, thus trivially holds $\Delta t = 1/m$, for all others relativistically $\Delta t > 1/m$.

The *second variation*[31] (which has no correspondence in current theories) varies the nodes $\mathbf{x}_k$. For this, it is needed to state, that for small $\delta\mathbf{x} << \mathbf{x}$ holds (see appendix)[32]

$$(\mathbf{x}+\delta\mathbf{x})^{-1} \approx \mathbf{x}^{-1} - \mathbf{x}^{-1}\delta\mathbf{x}\mathbf{x}^{-1}. \tag{12}$$

The variation of $\mathbf{x}_k$ influences only $\mathbf{v}_k$ and $\mathbf{v}_{k-1}$ (by their definition) and leads to

$$\delta\mathbf{v}_k = +\mathbf{v}_k\delta\mathbf{x}_k\mathbf{v}_k \quad \text{and} \quad \delta\mathbf{v}_{k-1} = -\mathbf{v}_{k-1}\delta\mathbf{x}_k\mathbf{v}_{k-1} \tag{13}$$

The variation of $\mathcal{L}$ in (7) is consequently (second line by circulation):

$$\begin{aligned} \delta\mathcal{L} &= \mathcal{T}(\mathbf{v}_k\delta\mathbf{x}_k\mathbf{v}_k P_k P_k^\dagger) - \mathcal{T}(\mathbf{v}_{k-1}\delta\mathbf{x}_k\mathbf{v}_{k-1}P_{k-1}P_{k-1}^\dagger) \\ &= \mathcal{T}(\delta\mathbf{x}_k(\mathbf{v}_k P_k P_k^\dagger \mathbf{v}_k - \mathbf{v}_{k-1}P_{k-1}P_{k-1}^\dagger\mathbf{v}_{k-1})). \end{aligned} \tag{14}$$

Again, this expression must vanish for arbitrary $\delta\mathbf{x}_k$, leading to

$$\mathbf{v}_k P_k P_k^\dagger \mathbf{v}_k \stackrel{!}{=} \mathbf{v}_{k-1}P_{k-1}P_{k-1}^\dagger\mathbf{v}_{k-1}, \tag{15}$$

Inserting equations (11) twice, results in $P_kP_k^\dagger = P_{k-1}P_{k-1}^\dagger = const.$. This is fulfilled by the condition $P_k = P_{k-1}S$, with an arbitrary matrix, that obeys $SS^\dagger = I$ (gauge invariance).
On the other hand, follows from equation (15):[33]

$$\mathbf{v}_k = \mathbf{v}_{k-1}, \tag{16}$$

that says, that the motion vector is constant over time, as it should be.

The result of above computations is, that the particle "moves" in jumps with a constant time-space vector $\mathbf{x}_{k+1} - \mathbf{x}_k = \Delta\mathbf{x}$, which is related to the particle wavelength by $\sqrt{|\Delta\mathbf{x}|} = 1/m$. The MINKOWSKI vector $\overline{\mathbf{v}_k} = const.$ is therefore to identify with the relativistic energy-impuls vector $\mathbf{p} = \varepsilon + \vec{p}$, where ε denotes the energy and it holds $|\mathbf{p}| = \varepsilon^2 - |\vec{p}|^2 = m^2$.
The spinor orientation does not have any influence on the motion, as to expect in the absence of an external field.

In any case, the time-steps that arise in these jumps are by orders too small to be visible in experiments (e.g. with ultrashort laser pulses). For an electron e.g. holds $\Delta t \approx 10^{-20}s$.

3.5 Stationary Case

This case describes bound states, e.g. an electron in an atom. I will show in the following, that it leads to the correct energy spectrum.

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[31] This is not to misinterprete as a *second order* variation.
[32] A simple proof is, to multiply the equation from the left (or right) with $(\mathbf{x}+\delta\mathbf{x})$.
[33] The other solution $\mathbf{v}_k = -\mathbf{v}_{k-1}$ would imply a step backwards in time.

The grid for this case is considered as "time invariant", i.e. it is claimed $\mathbf{x}_{i,k+1} - \mathbf{x}_{ik} = \tau$, where $\tau = real,\ \tau > 0$ is a constant time step.[34]
Only in this "periodic" case, the space components of the graph are constant over time (for all time indecees).
The space-like edges shall be pure space vectors (traceless matrices $\bar{\mathbf{x}} = -\mathbf{x}$).

Additionally, for all i, k the ansatz $P_{i,k+1} = P_{i,k}S$ is made[35] (i.e. $P_{i,k} = P_{i,1}S^{k-1}$) with a constant matrix S, obeying $SS^\dagger = I$ and $|S| = 1$.[36]

It follows $|P_{i,k}| = |P_{1,k}|, \quad P_{i,k+1}P_{i,k+1}^\dagger = P_{i,k}P_{i,k}^\dagger = \cdots = P_{i,1}P_{i,1}^\dagger = const.$ and $P_{i,k-1}P_{j,k}^\dagger = P_{i,k-1}S^\dagger P_{j,k-1}^\dagger = \cdots = P_{i,1}S^\dagger P_{j,1}^\dagger$.

The summands of $\mathcal{L}$ in (5) then become independent of the time index k, if also the external field is considered as time invariant: $\mathbf{A}_{i,k} = \mathbf{A}_{i,1}$. The index $k = 1$ can be dropped, also the summation over k can be omitted and one gets:

$$\begin{aligned} \mathcal{L} &= \sum_i \mathcal{T}((\frac{1}{\tau} + e\bar{\mathbf{A}}_i)P_iP_i^\dagger) + \frac{1}{2}\sum_{ij}\mathcal{T}((\mathbf{x}_i - \mathbf{x}_j)^{-1}(P_iS^\dagger P_j^\dagger + P_jSP_i^\dagger)) \\ &- 2m\sum_i \Re(|P_i|). \end{aligned} \tag{17}$$

Again, the double sum is to build only over edge-pairs (i, j).

To simplify the formulas, I introduce a set of auxiliary variables

$$\mathbf{u}_{ij} \stackrel{def}{=} (\mathbf{x}_i - \mathbf{x}_j)^{-1} = -\mathbf{u}_{ji}.$$

The antisymmetry of the factor $\mathbf{u}_{ij}$ in the double sum in i, j leads to a simplification, e.g. the summands for the pair $(1, 2)$ are:

$$P_1S^\dagger P_2^\dagger + P_2SP_1^\dagger - P_2S^\dagger P_1^\dagger - P_1SP_2^\dagger = P_1(S^\dagger - S)P_2^\dagger + P_2(S - S^\dagger)P_1^\dagger.$$

Any unit quaternion S can generally be represented with real λ and U as general, pure vectorial, unit quaternion ($U^\dagger = \bar{U} = -U$, $|U| = 1$)[37] as:

$$S = e^{\lambda U} = \cos\lambda + U\sin\lambda. \tag{18}$$

This gives $S - S^\dagger = 2U\sin\lambda$. Inserting this in (17) follows, that the double sum is proportional to $\sin\lambda$ (which is the only term containing λ). The extremal principle then requires (since λ is a free ansatz-parameter), that $\cos\lambda \stackrel{!}{=} 0$,

[34] Like above, it can be identified with the inverse energy of the state and its value follows from the equations below as the *eigenvalue*.

[35] Considering S beeing independent of the spatial index i is the standard method of "separating variables" (here time and space are to separate). In function form one would make e.g. the ansatz $\Psi(x,t) = \phi(x)\psi(t)$ and here S^k stands for the time dependency factor.

[36] These conditions hold for all *unit quaternions* S, which is equivalent to $S \in SU(2)$.

[37] U has 2 free real parameters and its general form is $U = \begin{pmatrix} i\sin\varphi, & \cos\varphi e^{i\chi} \\ \cos\varphi e^{-i\chi}, & -i\sin\varphi \end{pmatrix}$.

therefore $S = \pm U$ and $S^\dagger = -S$,[38] and equation (17) simplifies to (here also τ is replaced by the energy $\varepsilon = 1/\tau$)

$$\mathcal{L} = \sum_i \mathcal{T}((\varepsilon + e\bar{\mathbf{A}}_i)P_i P_i^\dagger) + \sum_{ij} \mathcal{T}(\mathbf{u}_{ij} P_j S P_i^\dagger) - 2m \sum_i \Re(|P_i|). \tag{19}$$

The variation of P_i is carried out like in the last section and leads to the "field equation" (a system of n linear equations for the $P_i,\ i = 1, \ldots, n$):[39]

$$(\varepsilon + e\bar{\mathbf{A}}_i)P_i + \sum_{ij} \mathbf{u}_{ij} P_j S = m\bar{P}_i^\dagger \tag{20}$$

This equation becomes equal to the DIRAC-equation for the stationary case, if the "operator" $\sum_{ij} \mathbf{u}_{ij}$ is replaced by the spatial derivative (∇-operator). This correspondence is shown in the appendix.[40]

Again, I consider a *second variation* of the grid points $\mathbf{x}_i$. The "equations of motion" derived with this method, result in the determination of the grid points. Again, this procedure has no counterpart in the present theories.
Please consider again, that this variation does *not affect* the spinors P_i.
In the next section I will show, that it produces the correct quantum states for the electron in COULOMB-potential.

For the variation of $\mathbf{x}_i$ in the sum (19), at first it is needed, that[41]

$$\delta\mathbf{A}_i = \delta\mathbf{A}(\mathbf{x}_i) = \frac{1}{2}\mathcal{T}(\delta\mathbf{x}_i\bar{\partial})\mathbf{A}_i, \tag{21}$$

where ∂ is the MINKOWSKIan differential operator (an explicit representation in matrix notation is given in the appendix).

The variation of $\mathbf{u}_{ij} = (\mathbf{x}_i - \mathbf{x}_j)^{-1}$ is again

$$\delta\mathbf{u}_{ij} = -\mathbf{u}_{ij}\delta\mathbf{x}_i\mathbf{u}_{ij} \quad \text{and} \quad \delta\mathbf{u}_{ji} = +\mathbf{u}_{ji}\delta\mathbf{x}_i\mathbf{u}_{ji}. \tag{22}$$

It results for the variation of $\mathbf{x}_i$, when another auxiliary variable $H_{ij} \stackrel{def}{=} P_i S P_j^\dagger$ (with $H_{ij}^\dagger = -H_{ji}$) is introduced for simplification (note, that in the sum i is fixed) [42]

$$\delta\mathcal{L} = \frac{e}{2}\mathcal{T}(\delta\mathbf{x}_i\bar{\partial})\mathcal{T}(\mathbf{A}_i P_i P_i^\dagger) + \sum_{ij} \mathcal{T}(\mathbf{u}_{ji}\delta\mathbf{x}_i\mathbf{u}_{ji}H_{ij} - \mathbf{u}_{ij}\delta\mathbf{x}_i\mathbf{u}_{ij}H_{ji}). \tag{23}$$

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[38] In the following one may use e.g. $S = U = \left(\begin{smallmatrix} i, & 0 \\ 0, & -i \end{smallmatrix}\right)$, the explicit form does not matter.

[39] Note, that the sum in this equation, in contrast to the sums above, is simple, since i is fixed.

[40] If one consideres this equation as a classical eigenvalue-problem for ε (given $\mathbf{x}_i$ and $\mathbf{A}_i$) it has, of course, at least n solutions ε_i and corresponding eigenvectors (at most $4n$, because every matrix-equation has actually 4 scalar equations).

[41] see appendix for a short explanation.

[42] the differential operator here operates only on the external field $\mathbf{A}$, of course, since P_i is considered as a constant.

From the demand $\delta\mathcal{L} = 0$ for all $\delta\mathbf{x}_i$ (with operations like in previous section), results the equation[43]

$$\frac{e}{2}\overline{\partial}\mathcal{T}(\mathbf{A}_i P_i P_i^\dagger) + \sum_{ij} \mathbf{u}_{ji}(H_{ij} + H_{ij}^\dagger)\mathbf{u}_{ji} = 0. \tag{24}$$

The combined solution of (20) and (24) is then the expected quantum state, which also determines ε, as it is to see in the following examples.

However, sometimes it is easier to use another method, that obviously leads to the same results. For all solutions of equation (20) follows, that $\mathcal{L} = 0$ holds. Then $\mathcal{L}(\varepsilon, p_1, p_2, \ldots) = 0$ is an implicit equation for ε (p_i subsumming all free variables, here as simple reals). Since $\mathcal{L}$ shall be extremal with respect to all other parameters p_i it follows $\dfrac{\partial\varepsilon}{\partial p_i} = 0$, so $\varepsilon(p_1, \ldots)$ itself must be extremal (usually minimal).

4 Electron in an Atom

In the usual approximation, the atom nucleus shows a COULOMB potential, leading to scalar $e\mathbf{A} = eV(r) = \frac{\alpha}{r}$, where $\alpha = e^2 \approx 1/137$ denotes the "finestructure constant" and $r = \sqrt{x^2 + y^2 + z^2}$ the EUCLIDian distance to the center.[44]

4.1 COULOMB-potential

To solve the equation (20) we first rewrite it for COULOMB-potential, by using the auxiliary parameters $\varepsilon_j \overset{def}{=} \varepsilon + \alpha/r_j$, and the same with conjugation[45]

$$\varepsilon_i P_i + \sum_{i\neq j} \mathbf{u}_{ij} P_j S = m\overline{P_i^\dagger} \quad \text{equals} \quad \varepsilon_i \overline{P_i^\dagger} - \sum_{i\neq j} \mathbf{u}_{ij} \overline{P_j^\dagger} S = m P_i.$$

By defining

$$P_i^+ \overset{def}{=} P_i + \overline{P_i^\dagger} \quad \text{and} \quad P_i^- \overset{def}{=} (P_i - \overline{P_i^\dagger})S \tag{25}$$

and addition/subtraction of both equations one gets:[46]

$$(\varepsilon_i - m)P_i^+ = -\sum_{i\neq j} \mathbf{u}_{ij} P_j^- \quad \text{and} \quad (\varepsilon_i + m)P_i^- = \sum_{i\neq j} \mathbf{u}_{ij} P_j^+. \tag{26}$$

[43] for the important special case, that $\mathbf{A}$ is time constant, $(\partial + \bar{\partial})\mathbf{A} = 0$ holds and therefore from (24) can be derived $\sum_{ij} \mathbf{u}_{ji}^2 \mathcal{T}(H_{ij} + H_{ij}^\dagger) = 0$, since $\mathbf{u}_{ji}^2 = scalar$.

[44] In matrix notation holds $r = \sqrt{-|\mathbf{x}|}$.

[45] consider $\overline{\mathbf{u}} = -\mathbf{u}$, $\mathbf{u}^\dagger = \mathbf{u}$ and $\overline{S^\dagger} = S$.

[46] Since P^+ and P^- by their definition obey: $\overline{(P^+)^\dagger} = P^+$ and $\overline{(P^-)^\dagger} = -P^-$ this is a *quaternionic* decomposition of P as $P = P^+ - P^- S$, where P^+ and iP^- are quaternions (see appendix). Since also $i\mathbf{u}$ is a quaternion, this set of equations (26) can represented with these algebraic entities.

The LAGRAGIAN sum (19) reads with this substitution:[47]

$$\mathcal{L} = \sum_i \big((\varepsilon_i - m)|P_i^+| - (\varepsilon_i + m)|P_i^-|\big) + \sum_{ij} \mathcal{T}(\overline{P_i^-}\mathbf{u}_{ij}P_j^+). \tag{27}$$

At this stage the SCHRÖDINGER-approximation is easily feasible, by setting $\varepsilon_i + m \approx 2m$ in (26) or (27). This is done in section 6. However, in the following sections I want to present precise results.

4.2 Ground State

At first, I start with the simplest case: the ground state in an atom, and will show, that the above formulas lead to the correct energy (and atom radius).
This state will be described with only two points $(n = 2)$[48] : $\mathbf{x}_1, \mathbf{x}_2$. Then exists only one edge $\mathbf{u}_{12} = (\mathbf{x}_1 - \mathbf{x}_2)^{-1} \stackrel{def}{=} \mathbf{u} = -\mathbf{u}_{21}$. However, as explained in the section F, this edge is counting *twice*, giving a factor of 2, so equation (26) reads:[49]

$$\begin{aligned} (\varepsilon_1 - m)P_1^+ &= -2\mathbf{u}P_2^- \qquad \text{and} \qquad (\varepsilon_1 + m)P_1^- = +2\mathbf{u}P_2^+, \\ (\varepsilon_2 - m)P_2^+ &= +2\mathbf{u}P_1^- \qquad \text{and} \qquad (\varepsilon_2 + m)P_2^- = -2\mathbf{u}P_1^+. \end{aligned} \tag{28}$$

In these four equations only the two spinor-pairs P_1^+, P_2^- and P_2^+, P_1^- are coupled, therefore eliminating the P_i^-, results in the pair of equations:

$$(\varepsilon_1 - m)(\varepsilon_2 + m)P_1^+ = 4\mathbf{u}^2P_1^+, \quad (\varepsilon_1 + m)(\varepsilon_2 - m)P_2^+ = 4\mathbf{u}^2P_2^+. \tag{29}$$

In these two equations the spinors P_i^+ are then freely variable and can be divided out (except for the two singular cases $P_1^+ = P_2^- = 0$ or $P_2^+ = P_1^- = 0$ resp.)[50] and one gets[51]

$$(\varepsilon_1 - m)(\varepsilon_2 + m) = 4\mathbf{u}^2, \quad (\varepsilon_1 + m)(\varepsilon_2 - m) = 4\mathbf{u}^2. \tag{30}$$

Consequently follows from $(\varepsilon_1 - m)(\varepsilon_2 + m) = (\varepsilon_1 + m)(\varepsilon_2 - m)$, that $\varepsilon_1 = \varepsilon_2$ must hold, i.e. $r_1 = r_2 \stackrel{def}{=} r$.
The resulting equation is

$$(\varepsilon + \frac{\alpha}{r})^2 - m^2 = 4\mathbf{u}^2. \tag{31}$$

[47] Of course, one also can derive again (26) from (27).

[48] It is easy to show, that for $n = 1$ no stationary solution exists.

[49] with $r_i \stackrel{def}{=} ||\mathbf{x}_i|| = \sqrt{-|\mathbf{x}_i|}$ and again $\varepsilon_i \stackrel{def}{=} \varepsilon + \frac{\alpha}{r_i}$

[50] The above decomposition on P into $P^{\pm}$ in (25) has the consequence that the LAGRANGian (27) becomes a sum of two terms: $\mathcal{L}_1(P_1^+, P_2^-, \varepsilon, \mathbf{x}_1, \mathbf{x}_2) + \mathcal{L}_2(P_2^+, P_1^-, \varepsilon, \mathbf{x}_1, \mathbf{x}_2)$, where the spinor-pairs must be viewed as varying independently. Therefore, these singular cases not have to be considered.
If one nevertheless computes these cases in full detail, eg. the first one, where only the second eq. of (30) holds, it turns out, however, that the resulting expression $\varepsilon(\mathbf{x}_1, \mathbf{x}_2)$ has only *one stationary point*, which is no extremum, but a saddle-point.

[51] The factors on both sides are simple reals. Consider again, that $\mathbf{u}$ is a traceless matrix by definition, so $\overline{\mathbf{u}} = -\mathbf{u}$ and $\mathbf{u}^2 = -|\mathbf{u}| \geq 0$.

Since $|\mathbf{x}_1| = |\mathbf{x}_2| = -r^2$ holds, by triangle formulas one gets: $-|\mathbf{x}_1 - \mathbf{x}_2| = 4(r^2 - h^2) \leq 4r^2$, with $h \leq r$ as height on the edge, so $4\mathbf{u}^2 = 1/(r^2 - h^2)$ and it results[52]

$$\varepsilon(r, h) = -\frac{\alpha}{r} \pm \sqrt{m^2 + \frac{1}{r^2 - h^2}}. \tag{32}$$

As explained above, the LAGRANGian extremal principle requires that this expression is to make stationary with respect to r and h, which after simple computations gives[53] immediately $h \stackrel{!}{=} 0$ and $r \stackrel{!}{=} \frac{\sqrt{1-\alpha^2}}{\alpha m} \approx \frac{1}{\alpha m}$ (BOHRs formula for the radius of the hydrogen atom) and finally the correct energy of the ground state:

$$\underline{\varepsilon = m\sqrt{1 - \alpha^2}}. \tag{33}$$

4.3 Space-Grid for the General State

The purpose of this section is, to present a general space grid, that is *stationary* together with the spinors. And I will show, that this represents the correct quantum states of an atom.

Therefore, I first consider a separation of variables, namely the radial variable r and angular variables (on the sphere). This separation is possible due to the symmetry of the COULOMB potential and is similar to usual procedures.

However, I want to emphasize here, that it should be possible to find *more general methods*, which do not rely on the assumption of *separability*, used below. I think, that once the edge scheme is fixed (i.e. which nodes are connected by edges), it can be proved, that the nodes are general stationary points. This was e.g. shown for the ground state in the last section, where it was forced by the equations, that both nodes have the same distance to the center.

The grid should consist of n spheres with the radii $r_i = r_1, .., r_n$, and all these spheres should have the same set of node normals. That means that every point of the grid can be represented as $\mathbf{x}_k = r_i \mathbf{p}_j$, where $\mathbf{p}_j$ are unit vectors: $|\mathbf{p}_j| = -1$.
Two points on different spheres $r_i \neq r_j$ also should only be connected by an edge, if they have the same spherical coordinates.

Again, the task is to find a stationary point for the LAGRANGian sum in (27):

$$\mathcal{L}(r_i, \mathbf{p}_i, P_i^+, P_i^-).$$

The separation ansatz now assumes, that also the spinors $P_i^\pm$ can be factorized, namely as

$$P_i^+ = f_i A_i \quad \text{and} \quad P_i^- = g_i \mathbf{p}_i A_i, \tag{34}$$

[52] In this formula r, h should not be misunderstood as usual variables: they get fixed values after using the extremal principle, also ε is then a constant, of course.

[53] only the + sign of the root gives for positive α (attractive potential) an extremum

where f_i and g_i should be real constants only depending on the radial index and A_i matrices, only depending on the angular index.

Considering that on radial edges holds $\mathbf{x}_i - \mathbf{x}_j = \mathbf{p}_i(r_i - r_j)$, introducing the auxiliary parameters $\varepsilon_i^{\pm} \overset{def}{=} \varepsilon_i \pm m$ and inserting the above into the sum (27) leads to (the summation labels R, S should denote summation over radial, resp. angular indicees):

$$\begin{aligned} \mathcal{L} &= \left(\sum_{k\in S} |A_k|\right)\left(\sum_{i\in R} \varepsilon_i^- f_i^2 + \varepsilon_i^+ g_i^2 + \sum_{ij\in R} \frac{f_i g_j - g_i f_j}{r_i - r_j}\right) \\ &+ \left(\sum_{kj\in S} \mathcal{T}(\bar{A}_k \bar{\mathbf{p}}_k (\mathbf{p}_k - \mathbf{p}_j)^{-1} A_j)\right)\left(\sum_{i\in R} \frac{f_i g_i}{r_i}\right) \end{aligned} \tag{35}$$

The usual separation idea is now, that the angular and radial dependent factors in both summands must be separable, that requires with some constant κ:

$$2\kappa \sum_S |A_i| \overset{!}{=} \sum_S \mathcal{T}(\bar{A}_i \bar{\mathbf{p}}_i (\mathbf{p}_i - \mathbf{p}_j)^{-1} A_j). \tag{36}$$

Then the sum can be decomposed into two independent factors $\mathcal{L} = \mathcal{L}_S \mathcal{L}_R$, where 2κ arises as eigenvalue in $\mathcal{L}_S$ and the radial factor $\mathcal{L}_R$ becomes:

$$\mathcal{L}_R = \sum_i (\varepsilon_i^- f_i^2 + \varepsilon_i^+ g_i^2) - 2\kappa \sum_i \frac{f_i g_i}{r_i} + \sum_{j\neq i} \frac{f_i g_j - g_i f_j}{r_i - r_j}. \tag{37}$$

The solution of the angular part $\mathcal{L}_S$ is given in the appendix, section F.

4.4 Solution of the Radial Equations

By variating the f_i, g_i in (37) one gets:[54]

$$\varepsilon_i^- f_i = \frac{\kappa}{r_i} g_i - \sum_{j\neq i} \frac{g_j}{r_i - r_j} \quad \text{and} \quad \varepsilon_i^+ g_i = \frac{\kappa}{r_i} f_i + \sum_{j\neq i} \frac{f_j}{r_i - r_j}. \tag{38}$$

At this point, I want to emphasize the correspondence to the radial differential equations, derived from DIRACs-equation, with similar presumptions, namely they read: $\varepsilon^- f = \frac{\kappa}{r} g - g'$, $\varepsilon^+ g = \frac{\kappa}{r} f + f'$ (see e.g. [8]).
The detailled discussion of this and also the connection of the both associated LAGRANGians is given in the appendix.

The *second variation*, which considers the r_i, additionally gives (for all r_i)[55]

$$\frac{d\mathcal{L}}{dr_i} = -\frac{\alpha}{r_i^2}(f_i^2 + g_i^2) + 2\kappa \frac{f_i g_i}{r_i^2} - 2\sum_{j\neq i} \frac{f_i g_j - g_i f_j}{(r_i - r_j)^2} \overset{!}{=} 0. \tag{39}$$

[54] Note, that the sums are only over the radial index, from here on.
[55] Consider, that $d\varepsilon_i^{\pm}/dr_i = -\alpha/r_i^2$ and the double sum contains each term twice.

The equations (38) set up a system of linear equations, which can be considered as eigenvalue problem for ε (if all r_i are fixed). Together with (39) they form a set of $3n$ equations for the $3n+1$ variables $r_i, f_i, g_i, \varepsilon$.[56]
Since the first system is linear in f_i, g_i and the second bilinear, however, they are normalizable, consequently the number of equations equals the number of variables, indicating that only discrete solutions exist.

For $n = 1$ the solution can be derived directly, giving (correctly)[57]

$$\varepsilon = \frac{m}{\kappa}\sqrt{\kappa^2 - \alpha^2}, \quad r_1 = \frac{\kappa}{\alpha m}\sqrt{\kappa^2 - \alpha^2}. \tag{40}$$

For the general case, it turns out, that a simple linear ansatz for the f_i, g_i, where a, b, c, d are real constants

$$f_i = a + br_i \quad \text{and} \quad g_i = c + dr_i, \tag{41}$$

and a set of r_i, obeying the equations (with two parameters λ, γ)[58]

$$\sum_{j \neq i} \frac{1}{r_i - r_j} = \lambda - \frac{\gamma}{r_i} \tag{42}$$

gives a solution which results (after longish computations) in the correct formula for the energy levels, where $n_r = n - 1$ is the radial quantum number (see e.g. [8], p. 126):[59]

$$\Big(\frac{m}{\varepsilon}\Big)^2 = 1 + \Big(\frac{\alpha}{\sqrt{\kappa^2 - \alpha^2} + n_r}\Big)^2. \tag{43}$$

5 Electron under LORENTZ-Force

This section is intended, to demonstrate the working of the method for one non-stationary case.[60]

I consider here the same case as in eq. (7), except that also an electromagnetic field is present, i.e. again with $n = 1$ (no space-like edges) and

[56] From here on, n denotes the number of spheres, not nodes.

[57] Consider from (38): $\varepsilon_1^- f_1 = \frac{\kappa}{r_1} g_1$, and $\varepsilon_1^+ g_1 = \frac{\kappa}{r_1} f_1$ and from (39) $\alpha(f_1^2 + g_1^2) = 2\kappa f_1 g_1$. This system of 3 equations has only the above solution.

[58] These equations are related to LAGUERRE-polynoms, and discussed in the appendix.

[59] The parameters are then determined as $\gamma = \sqrt{\kappa^2 - \alpha^2}$ and $\lambda = \sqrt{m^2 - \varepsilon^2}$.

[60] To tackle problems of this type as initial value problem (e.g. numerically), one should consider the following method. Suppose the three consecutive points $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ are used (and the associated spinors P_1, P_2). Then the variation equations for the inner point $\mathbf{x}_2$ and P_1, P_2, (45, 47) are used, building a set of 3 implicit equations. In this set, the initial values of $\mathbf{x}_1, \mathbf{x}_2, P_1$ are inserted, which eventually results in the values for $\mathbf{x}_3, P_2$, and so forth.

$\mathbf{v}_k \overset{def}{=} (\mathbf{x}_{k+1} - \mathbf{x}_k)^{-1}$.[61]

$$\mathcal{L} = \sum_k \mathcal{T}((\mathbf{v}_k + \frac{e}{2}(\bar{\mathbf{A}}_{k+1} + \bar{\mathbf{A}}_k))P_k P_k^\dagger) - 2m \sum_k \Re(|P_k|). \tag{44}$$

The "field equations" become similarly:

$$(\mathbf{v}_k + \frac{e}{2}(\bar{\mathbf{A}}_{k+1} + \bar{\mathbf{A}}_k))P_k = m\overline{P_k^\dagger}. \tag{45}$$

By taking the determinant on both sides of this equation immediately follows, that $|P_k|$ must be real[62] and consequently it must hold for all k (it is closely related to the conservation of energy):

$$|\mathbf{v}_k + \frac{e}{2}(\bar{\mathbf{A}}_{k+1} + \bar{\mathbf{A}}_k)| = m^2 = const. \tag{46}$$

One remarkable consequence of this simple formula is, that regardless of the history of a particle, in case of vanishing vector potential, in its rest frame always holds $\Delta t = 1/m$.[63]

The *second variations* (for $\mathbf{x}_k$) result in:[64]

$$\mathbf{v}_k P_k P_k^\dagger \mathbf{v}_k - \mathbf{v}_{k-1} P_{k-1} P_{k-1}^\dagger \mathbf{v}_{k-1} + \frac{e}{4}\bar{\partial}\mathcal{T}(\bar{\mathbf{A}}_k(P_k P_k^\dagger + P_{k-1}P_{k-1}^\dagger)) \overset{!}{=} 0. \tag{47}$$

Please, consider again, that the set of equations (45) and (47) must be solved simultaneously.
By multiplying (45) from the right with $P_k^\dagger$ and $(\mathbf{v}+e\mathbf{A})^{-1}$ from left one gets[65]

$$\begin{aligned} P_k P_k^\dagger &= m|P_k|(\mathbf{v}_k + \frac{e}{2}(\bar{\mathbf{A}}_{k+1} + \bar{\mathbf{A}}_k))^{-1} \\ &\approx m|P_k|(\mathbf{v}_k^{-1} - \mathbf{v}_k^{-1}\frac{e}{2}(\bar{\mathbf{A}}_{k+1} + \bar{\mathbf{A}}_k)\mathbf{v}_k^{-1}). \end{aligned} \tag{48}$$

Inserting this and the corresponding term for $P_{k-1}P_{k-1}^\dagger$ in (47) and omitting terms $\sim e^2\mathbf{A}^2$ gives (after division by m):

$$\begin{aligned} |P_k|(\mathbf{v}_k - \frac{e}{2}(\bar{\mathbf{A}}_{k+1} + \bar{\mathbf{A}}_k)) \quad &- \quad |P_{k-1}|(\mathbf{v}_{k-1} - \frac{e}{2}(\bar{\mathbf{A}}_k + \bar{\mathbf{A}}_{k-1})) \\ +\frac{e}{4}\bar{\partial}\mathcal{T}(\bar{\mathbf{A}}_k(|P_k|\mathbf{v}_k^{-1} \quad &+ \quad |P_{k-1}|\mathbf{v}_{k-1}^{-1})) = 0. \end{aligned} \tag{49}$$

[61] Again this sum is obviously invariant under the "local" transformations $P_k \to P_k S_k$, when $S_k S_k^\dagger = 1$ and $|S_k| = 1$. I.e. the spinors P_k are determined only up to these factors by the following equations. This is a partial analogy to gauge invariance of standard DIRAC theory, except the vector field $\mathbf{A}$ is not transformed here.

[62] consider $|\mathbf{v} + e\mathbf{A}||P| = m^2|P|^*$ and $|\mathbf{u}| = real$ for any HERMITEan $\mathbf{u}$.

[63] The equation, however, reveals some important new issues:
E.g. adding a constant offset to $\mathbf{A}$ (which does not affect the classical LORENTZ-force) here changes the discretization and thus modifies the results. It seems, that apparently no full gauge invariance can be derived for this model. For small fields, however, the results are equal to the classical theory.

Then for example, consider the simplest case: a resting particle in scalar potential $\mathbf{A} = U(\mathbf{x})$. Then eq. (46) reads: $(\frac{1}{\Delta t} + U)^2 = m^2$ i.e. $\Delta t = \frac{1}{|m| - U}$. Since $\Delta t > 0$ is supposed, only the range $-\infty < U < |m|$ for the external field is possible.

[64] consider again $\delta\mathbf{A}_k = \frac{1}{2}\mathcal{T}(\delta\mathbf{x}_k\bar{\partial})\mathbf{A}_k$

[65] if the approximation of small field $|e\mathbf{A}| << |\mathbf{v}|$ is used.

Reordering gives (after a bar-operation):

$$\begin{aligned} |P_k|(\bar{\mathbf{v}}_k - \frac{e}{2}(\mathbf{A}_{k+1} \quad + \quad \mathbf{A}_k) + \frac{e}{4}\partial\mathcal{T}(\bar{\mathbf{A}}_k\mathbf{v}_k^{-1})) \\ = |P_{k-1}|(\bar{\mathbf{v}}_{k-1} - \frac{e}{2}(\mathbf{A}_k \quad + \quad \mathbf{A}_{k-1}) - \frac{e}{4}\partial\mathcal{T}(\bar{\mathbf{A}}_k\mathbf{v}_{k-1}^{-1})). \end{aligned} \tag{50}$$

Now with $\mathbf{v}_k^{-1} = \mathbf{x}_{k+1} - \mathbf{x}_k$ (by definition) the approximations are used:[66]

$$\mathbf{A}_{k+1} \approx \mathbf{A}_k + \frac{1}{2}\mathcal{T}(\mathbf{v}_k^{-1}\bar{\partial})\mathbf{A}_k \quad \text{and} \quad \mathbf{A}_{k-1} \approx \mathbf{A}_k - \frac{1}{2}\mathcal{T}(\mathbf{v}_{k-1}^{-1}\bar{\partial})\mathbf{A}_k \tag{51}$$

resulting in

$$\begin{aligned} |P_k|(\bar{\mathbf{v}}_k - e\mathbf{A}_k \quad - \quad \frac{e}{4}\mathcal{T}(\mathbf{v}_k^{-1}\bar{\partial})\mathbf{A}_k) + \frac{e}{4}\partial\mathcal{T}(\bar{\mathbf{A}}_k\mathbf{v}_k^{-1})) \\ = |P_{k-1}|(\bar{\mathbf{v}}_{k-1} - e\mathbf{A}_k \quad + \quad \frac{e}{4}\mathcal{T}(\mathbf{v}_{k-1}^{-1}\bar{\partial})\mathbf{A}_k - \frac{e}{4}\partial\mathcal{T}(\bar{\mathbf{A}}_k\mathbf{v}_{k-1}^{-1})). \end{aligned} \tag{52}$$

Now the equation for the fieldtensor F (at point $\mathbf{x}_k$) is used (see appendix B), which for any $\mathbf{u}$ obeys: $\mathbf{u}F + F^\dagger\mathbf{u} = \mathcal{T}(\bar{\partial}\mathbf{u})\mathbf{A} - \partial\mathcal{T}(\mathbf{A}\bar{\mathbf{u}})$ giving

$$\begin{aligned} |P_k|(\bar{\mathbf{v}}_k - e\mathbf{A}_k \quad - \quad \frac{e}{4}(\mathbf{v}_k^{-1}F_k + F_k^\dagger\mathbf{v}_k^{-1})) \\ = |P_{k-1}|(\bar{\mathbf{v}}_{k-1} - e\mathbf{A}_k \quad + \quad \frac{e}{4}(\mathbf{v}_{k-1}^{-1}F_k + F_k^\dagger\mathbf{v}_{k-1}^{-1})). \end{aligned} \tag{53}$$

Since one cannot generally claim $|P_k| = |P_{k-1}|$ (which case could be easily solved), the symmetrical ansatz (which is always possible, of course) with a new real variable λ: $|P_k| = 1+\lambda, |P_{k-1}| = 1-\lambda$ is used. Also, the centered difference $\mathbf{q} \stackrel{def}{=} \mathbf{v}_k^{-1} + \mathbf{v}_{k-1}^{-1} = \mathbf{x}_{k+1} - \mathbf{x}_{k-1}$ is used. Then one gets:[67]

$$(1+\lambda)\bar{\mathbf{v}}_k - (1-\lambda)\bar{\mathbf{v}}_{k-1} = \frac{e}{4}(\mathbf{q}F_k + F_k^\dagger\mathbf{q}). \tag{54}$$

To determine λ, this equation is multiplied (from right) with $\bar{\mathbf{q}} = \bar{\mathbf{v}}_k^{-1} + \bar{\mathbf{v}}_{k-1}^{-1}$ and then is taken the trace, so the right-hand side vanishes (since $F + \bar{F} = 0$). It remains

$$\mathcal{T}((1+\lambda)(1+\bar{\mathbf{v}}_k\bar{\mathbf{v}}_{k-1}^{-1}) - (1-\lambda)(1+\bar{\mathbf{v}}_{k-1}\bar{\mathbf{v}}_k^{-1})) = 0. \tag{55}$$

Then, with $\mathbf{a} \stackrel{def}{=} \bar{\mathbf{v}}_k - \bar{\mathbf{v}}_{k-1}$ and another auxiliary matrix $B \stackrel{def}{=} \bar{\mathbf{v}}_k\bar{\mathbf{v}}_{k-1}^{-1} = 1 + \mathbf{a}\bar{\mathbf{v}}_{k-1}^{-1}$, one gets:

$$(1+\lambda)\mathcal{T}(1+B) = (1-\lambda)\mathcal{T}(1+B^{-1}) \quad \text{i.e.} \quad \lambda = \frac{\mathcal{T}(B^{-1}) - \mathcal{T}(B)}{4 + \mathcal{T}(B^{-1}) + \mathcal{T}(B)}. \tag{56}$$

[66] see appendix, chapter "Differential Calculus" for explanation.

[67] since $|\lambda| \ll 1$ is supposed to be small, only the dominant term $\sim \lambda$ is considered, which is $\bar{\mathbf{v}}$

With $\mathcal{T}(B^{-1}) = \frac{\mathcal{T}(B)}{|B|}$ and $|B| = \frac{|\mathbf{v}_k|}{|\mathbf{v}_{k-1}|}$[68] and the approximation $\mathcal{T}(B) \approx 2$ follows $\lambda \approx \frac{|\mathbf{v}_{k-1}|-|\mathbf{v}_k|}{4|\mathbf{v}_k|}$.

To state the approximation of LORENTZ-force of eq. (54) it remains to explain, that the relativistic velocity vector $\mathbf{u} = d\mathbf{x}/d\tau = \dot{\mathbf{x}}$ is discretized as[69] $\mathbf{u} = (\mathbf{x}_{k+1} - \mathbf{x}_{k-1})/\sqrt{|\mathbf{x}_{k+1} - \mathbf{x}_{k-1}|} \approx \frac{m}{2}\mathbf{q}$ i.e. $\underline{\mathbf{q} \approx \frac{2}{m}\mathbf{u}}$ and $\mathbf{a}$ is actually a discretized acceleration vector:

$$\begin{aligned} \mathbf{a} = \bar{\mathbf{v}}_k - \bar{\mathbf{v}}_{k-1} &= |\mathbf{v}_k|(\mathbf{x}_{k+1} - \mathbf{x}_k) - |\mathbf{v}_{k-1}|(\mathbf{x}_k - \mathbf{x}_{k-1}) \\ &\approx \frac{\mathbf{x}_{k+1} - 2\mathbf{x}_k + \mathbf{x}_{k-1}}{(\Delta\tau)^2} \approx \frac{d^2\mathbf{x}}{d\tau^2}. \end{aligned} \tag{57}$$

Finally from eq. (54) results the equation of LORENTZ-force (see appendix) with small corrections:[70]

$$\underline{\mathbf{a} = \frac{e}{2m}(\mathbf{u}F_k + F_k^\dagger \mathbf{u})} - 2\frac{\lambda}{m}\mathbf{u}. \tag{58}$$

6 SCHRÖDINGER-Approximation and "HAMILTON-Sum"

This section shall demonstrate, that also a *discrete form* of the classical stationary SCHRÖDINGER equation and its associated HAMILTONian can be derived as approximation from the above discrete DIRAC formalism. This approximation is always possible for electrons in weak electromagnetic fields.[71]

I start with equation (26) from section 4.1, which represents a bound state of an electron, but here in a general electric potential field $V(\mathbf{x})$ (real scalar, time independent) with $V_i \overset{def}{=} V(\mathbf{x}_i)$:[72]

$$(\varepsilon + V_i - m)P_i^+ = -\sum_j \mathbf{u}_{ij}P_j^- \quad \text{and} \quad (\varepsilon + V_i + m)P_i^- = \sum_j \mathbf{u}_{ij}P_j^+. \tag{59}$$

As mentioned, herein the SCHRÖDINGER-approximation is easily feasible, by setting $\varepsilon + V_i + m \approx 2m$ in the second equation.[73] Then P_i^- can be expressed directly with it:

$$P_i^- \approx \frac{1}{2m}\sum_j \mathbf{u}_{ij}P_j^+. \tag{60}$$

[68] consider from eq. (46) $|\mathbf{v}_k + \frac{e}{2}(\bar{\mathbf{A}}_{k+1} + \bar{\mathbf{A}}_k)| = |\mathbf{v}_{k-1} + \frac{e}{2}(\bar{\mathbf{A}}_k + \bar{\mathbf{A}}_{k-1})|$ $(= m^2)$ and $|e\mathbf{A}| \ll |\mathbf{v}|$ thus $|\mathbf{v}_k| \approx |\mathbf{v}_{k-1}|$ holds.

[69] centered around $\mathbf{x}_k$, using $\Delta\tau = \sqrt{|\mathbf{x}_{k+1} - \mathbf{x}_{k-1}|} = \sqrt{|\mathbf{v}_k^{-1} + \mathbf{v}_{k-1}^{-1}|} \approx \sqrt{4|\mathbf{v}_k^{-1}|} \approx 2/m$.

[70] The correction term resembles a corresponding term in DIRACs motion equation, which reads in this notation and scaling: $\frac{e^2}{6\pi m}(\dot{\mathbf{a}} - \mathbf{u}|\mathbf{a}|)$ (see e.g. [6], p. 173)

[71] The way of deriving this approximation from DIRAC equation is similar to standard QM.

[72] and again $\mathbf{u}_{ij} \overset{def}{=} (\mathbf{x}_i - \mathbf{x}_j)^{-1}$ for the space-edges

[73] This is the usual approximation method for small energy, since $\varepsilon \approx m$ and $V \ll m$

Inserting this in the first of (59), gives with $E \stackrel{def}{=} \varepsilon - m$ as energy:[74]

$$(E + V_i)P_i^+ = -\frac{1}{2m}\sum_{jk} \mathbf{u}_{ij}\mathbf{u}_{jk}P_k^+. \tag{61}$$

Please note, that the double-sum is to build over all edge-pairs (i, j) and (j, k). This is still a *matrix equation*. To get a *scalar* equation from it, one adds the adjuncted, resulting in a scalar expression:[75]

$$(E + V_i)(P_i^+ + \bar{P}_i^+) = -\frac{1}{2m}\sum_{jk}(\mathbf{u}_{ij}\mathbf{u}_{jk}P_k^+ + \bar{P}_k^+\mathbf{u}_{kj}\mathbf{u}_{ji}),$$

and then drops the vector part of P_k^+ in the r.h.s. (ignoring all spin-effects), by setting it a real scalar $\psi_k \stackrel{def}{=} P_k^+ = \bar{P}_k^+$.
The result is a discretized form of the stationary SCHRÖDINGER-equation:

$$(E + V_i)\psi_i = -\frac{1}{2m}\sum_{jk}\frac{1}{2}(\mathbf{u}_{ij}\mathbf{u}_{jk} + \mathbf{u}_{kj}\mathbf{u}_{ji})\psi_k. \tag{62}$$

The sum $\frac{1}{2}\sum_{jk}(\mathbf{u}_{ij}\mathbf{u}_{jk} + \mathbf{u}_{kj}\mathbf{u}_{ji})\psi_k$ there represents the second order partial derivation operator $\Delta\psi_k$[76] at the point $\mathbf{x}_i$.

One can also easily define a "HAMILTONian-sum", from which the above SCHRÖDINGER-equation (62) can be derived again (by variation of all ψ_k):[77]

$$H(\psi_i, \mathbf{x}_i) = \sum_i (E + V_i)\psi_i^2 + \frac{1}{2m}\sum_{ijk}\mathbf{u}_{ij}\mathbf{u}_{jk}\psi_k\psi_i \tag{63}$$

This sum obviously corresponds to the classical HAMILTONian for the stationary case.[78]

6.1 General Considerations about Ground States

At first, I want to discuss the solution for the ground states of any potential V, which is described here with $n = 2$ nodes.
Then one has only one edge with $\mathbf{u} \stackrel{def}{=} \mathbf{u}_{12} = (\mathbf{x}_1 - \mathbf{x}_2)^{-1} = -\mathbf{u}_{21}$ and two equations:

$$(E + V_1)\psi_1 = -\frac{1}{2m}\mathbf{u}_{12}\mathbf{u}_{21}\psi_1 = \frac{\mathbf{u}^2}{2m}\psi_1 \quad \text{and} \quad (E + V_2)\psi_2 = \frac{\mathbf{u}^2}{2m}\psi_2. \tag{64}$$

[74] in many textbooks the potential energy $U = -V$ is used instead of V in the formulas
[75] consider that E, V_i are scalars and $\bar{\mathbf{u}}_{jk} = -\mathbf{u}_{jk}$ and $\mathbf{u}_{kj} = -\mathbf{u}_{jk}$ holds.
[76] It is always scalar and real, of course.
[77] Of course, it it also possible to derive this HAMILTONian directly from the LAGRANGian sum, with the same assumptions.
[78] The proof, that the triple sum is always a real scalar, is simple when again the hermitecity and antisymmetry of the $\mathbf{u}_{ij} = \mathbf{u}_{ij}^\dagger = -\mathbf{u}_{ji}$ is used, e.g. $(\mathbf{u}_{12}\mathbf{u}_{23})^\dagger = \mathbf{u}_{23}\mathbf{u}_{12} = \mathbf{u}_{32}\mathbf{u}_{21}$.

It follows $E + V_1 = E + V_2 = \frac{\mathbf{u}^2}{2m}$, i.e. at first one can conclude $V_1 \stackrel{!}{=} V_2$.
Please note, that for every MINKOWSKIan pure space-vector $\mathbf{u}$ (with $\bar{\mathbf{u}} = -\mathbf{u}$) holds $\mathbf{u}^2 = -|\mathbf{u}| > 0$, therefore $E > -V_{1,2}$
Also notable is the decoupling of ψ_1, ψ_2 in equation (64), meaning that their values are independent.[79]

However, in contrast to the case of COULOMB-potential discussed below: if there exists a stationary point $\mathbf{x}_0$ of the potential (with $\frac{\partial V(\mathbf{x}_0)}{\partial \mathbf{x}} = 0$), then also a solution with only one node ($n = 1$, no edge) is possible, which then would have the energy $E = -V(\mathbf{x}_0)$.
These solutions do not have counterparts in current QM. To exclude them, there must be a principle, that excludes stationary solutions with $n = 1$. At the moment I cannot see, what this can be.

6.2 Ground State in COULOMB-potential

The COULOMB-field (of an atom nucleus) is (with $r = ||\mathbf{x}||$ as euclidian distance)

$$V(\mathbf{x}) = \frac{\alpha}{r}. \tag{65}$$

Then (again from $V_1 = V_2$) directly follows $r_1 = r_2 = r$. As explained above, in contrast to the one-dimensional case, the edge is counting *twice* again, so one gets

$$E = -\frac{\alpha}{r} + \frac{4\mathbf{u}^2}{2m} \tag{66}$$

By setting $1/\mathbf{u}^2 = (\mathbf{x}_1 - \mathbf{x}_2)^2 = 4(r^2 - h^2)$ results:[80]

$$E(r, h) = -\frac{\alpha}{r} + \frac{1}{2m(r^2 - h^2)}. \tag{67}$$

The condition $\frac{\partial E}{\partial h} = 0$ then gives $h = 0$, and $\frac{\partial E}{\partial r} = 0$ gives $r = 1/\alpha m$ (atom radius) and finally the energy of the ground state of hydrogen:

$$E = -m\frac{\alpha^2}{2}. \tag{68}$$

6.3 Quantum Harmonic Oscillator

This section is included, to give readers the most simple testcase of the discrete theory. The one-dimensional harmonic oscillator has the field (with usual scale factor):

$$V(x) = -\frac{m}{2}\omega^2 x^2. \tag{69}$$

[79] This does not hold for the exact solution, given in chapter 4.2., there the spinor P_k cannot vanish at any point k.
[80] With simple triangle formula for the triangle $(\mathbf{x}_1, \mathbf{0}, \mathbf{x}_2)$, with h as height and $h \leq r$.

Here for simplification is set $m = \omega = 1$, giving from (63) the "HAMILTONian sum":[81]

$$H(\psi_i, x_i) = \sum_i (E - \frac{1}{2}x_i^2)\psi_i^2 + \frac{1}{2}\sum_{ijk} \frac{\psi_i\psi_k}{(x_i - x_j)(x_j - x_k)}. \tag{70}$$

Here all node-pairs (i, j) shall be connected by one edge, with a total of $\frac{n(n-1)}{2}$ edges.
The "field equation" (by variation of ψ_m) results in n eqn.

$$2(E - \frac{1}{2}x_m^2)\psi_m + \sum_{jk} \frac{\psi_k}{(x_m - x_j)(x_j - x_k)} \stackrel{!}{=} 0. \tag{71}$$

The variation (differentiation) of (15) by $x_m, m = 1, .., n$ gives also n eqn:

$$\begin{aligned} -x_m\psi_m^2 \quad &- \quad \frac{1}{2}\sum_{jk} \frac{\psi_m\psi_k}{(x_m - x_j)^2(x_j - x_k)} + \frac{1}{2}\sum_{ik} \frac{\psi_i\psi_k}{(x_i - x_m)^2(x_m - x_k)} \\ &- \quad \frac{1}{2}\sum_{ik} \frac{\psi_i\psi_k}{(x_i - x_m)(x_m - x_k)^2} + \frac{1}{2}\sum_{ij} \frac{\psi_i\psi_m}{(x_i - x_j)(x_j - x_m)^2} \stackrel{!}{=} 0. \end{aligned}$$

This can be simplified to:[82]

$$-x_m\psi_m^2 - \sum_{jk} \frac{\psi_m\psi_k}{(x_m - x_j)^2(x_j - x_k)} + \sum_{jk} \frac{\psi_j\psi_k}{(x_j - x_m)^2(x_m - x_k)} \stackrel{!}{=} 0 \tag{72}$$

These $2n$ equations (71, 72) are to solve with $2n$ variables (ψ_i, x_i). Since it is wellknown, that HERMITE-polynoms are the eigenfunctions of the classical quantum harmonic oscillator, it is suggested using them to find a solution. And indeed, it is simple to prove the following solution with their help.[83]

I will show in the following, that with x_i as zeros of these HERMITE-polynoms, and the most simple ansatz for the ψ_i: $\underline{\psi_i = a}$ (an arbitrary constant) all $2n$ equations are fulfilled, so this is actually *a stationary point* of $H(\psi_k, x_k)$.

The zeros of HERMITE-polynoms $(x_1, \ldots, x_n)$ obey the implicit equation set[84]

$$\sum_{i=1, i\neq k}^{n} \frac{1}{x_k - x_i} = x_k \tag{73}$$

[81] Consider e.g. the one-dimensional case with $\mathbf{x} = \binom{0,x}{x,0}$ $(y = z = 0)$. Then the $\mathbf{u}_{ij} = (\mathbf{x}_i - \mathbf{x}_j)^{-1}$ all commute, and their products $\mathbf{u}_{ij}\mathbf{u}_{jk} = \frac{1}{(x_i - x_j)(x_j - x_k)}$ are always simple scalars

[82] by the reassignement of the sum indicees in the 4. sum $i \to k$ (equals $-$ 1. sum) and of the 3.rd sum $i \leftrightarrow k$ (equals $-$ 2.) and then $i \to j$

[83] Possibly this is not the only solution, also if permutations of the x_i are considered.

[84] Please note, that the x_i are uniquely determined by (73) (up to permutations, of course). The first few zeros can be computed explicitely, e.g. for $\underline{n = 1}$: $x_1 = 0$, for $\underline{n = 2}$: $x_{1,2} = \pm\sqrt{\frac{1}{2}}$, for $\underline{n = 3}$: $x_1 = -\sqrt{\frac{3}{2}}, x_2 = 0, x_3 = \sqrt{\frac{3}{2}}$.

This is easy to prove with the methods given in appendix E: "Orthogonal Polynoms".[85]
The proof of (72) is then simple (factors a^2 dropped) with reordering both double sums:

$$\sum_j \frac{1}{(x_m - x_j)^2} \left(\sum_k \frac{1}{x_m - x_k} - \sum_k \frac{1}{x_j - x_k} \right) = \sum_j \frac{x_m - x_j}{(x_m - x_j)^2} = \underline{x_m}.$$

From the above implicit sum formulas (73) for the x_i, one can easily derive[86]

$$\sum_{i=1}^{n} x_i = 0 \quad \text{and} \quad \sum_{i \neq k}^{n} \frac{x_i}{x_k - x_i} = x_k^2 - (n-1).$$

The double sum in (71) then becomes:

$$\sum_{jk} \frac{a}{(x_m - x_j)(x_j - x_k)} = \sum_j \frac{a x_j}{(x_m - x_j)} = a(x_m^2 - (n-1))$$

and one gets:

$$\underline{E = \frac{n-1}{2}} \tag{74}$$

This formula reproduces the wellknown energy levels of the quantum harmonic oscillator, if the restriction $n = even$ is made.[87]
However, it is not clear yet, which physical principle excludes the other solutions (for $n = odd$).

7 Conclusions and Outlook

Here I presented a new discrete view to quantum mechanics, where the continuous wave functions are replaced by a space-time graph with attached constant spinors and the differential equations by discrete, algebraic equations. These equations are derived from a general "LAGRANGian sum" over the graph.

The remarkable new idea is, that the *graph nodes* are not to be arbitrary set, but determined by the variation principle for *the same sum*.
Since the graph is a MINKOWSKI space-time graph, this includes the *time steps* (which are for stationary cases then determined by the energy eigenvalue of the state) and gives also a valid description of *particle movement* (nonstationary case).

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[85] They have the generating differential equation (see eq. (A.30)): $y'' - 2xy' + \lambda y = 0$, i.e. $u(x) = 1$, $v(x) = -2x$, $\frac{v}{u} = -2x$.
[86] e.g. with $\sum_i \frac{x_i}{x_k - x_i} = \sum_i \frac{x_i - x_k + x_k}{x_k - x_i} = \sum_{i \neq k} (-1 + \frac{x_k}{x_k - x_i}) = -(n-1) + x_k^2$.
[87] Consider the units $\hbar = \omega = 1$

With this model many classical problems of quantum mechanics are solved and give the expected results. (However, some of the solutions do not have a correspondence in classical QM. It is not yet clear, which *physical principle* suppresses them.)
It is thus my hope, that this model can make the wave function obsolete (similar to the *light aether*, that became obsolete by the theory of Special Relativity), and *all quantum phenomena can be described by a finite number of numbers, as an algebraic theory*, like A. EINSTEIN suggested.

However, there remain also many unanswered questions:
One principal task is, to introduce real dynamic behaviour into the theory, e.g. to describe emission and absorption processes. Then also the model of a photon should arise. The space-time graph for a photon, as massless particle must be described differently, however, since the time-like edges must be replaced by *light-like* edges, with $|\Delta\mathbf{x}| = 0$.

These processes could be probably modelled with bifurcations and combinations of the graph. In general, due to the implicit character of the formulas, this should be possible, because they may have more than one solution.

Additionally, the usage of the electromagnetic vector potential in the theory, can only be seen as an approximation of interactions with (virtual) photons. This however, would imply significant changes of the variational principle.[88]

Another interesting aspect is the question, if it is possible, to set one primary entity (between spinors and MINKOWSKIan vectors), from which the other can be constructed as derivation. Apparently, this can be only the spinor part.
However, it is to expect that this question can only be solved in a more general framework, which I suppose to be a discrete theory at the PLANK-scale level (*quantum gravity*), that will have a quite different concept of space-time. From that, the presented theory will arise as approximation.

Other important tasks are:

- Is it possible, to simplify the LAGRANGian sum (5), e.g. combine time-like and space-like terms, and find some kind of deeper explanation for it?
- Can gauge invariance represented better? What happens for strong fields, where $||e\mathbf{A}|| \sim m$?
- How are many-particle systems described? This should be possible, of course, by defining a composed LAGRANGian .
- How are antiparticles described in this theory?

[88]However, it should be stressed, that for the most important case (COULOMB-potential), there exists a striking correnspondence between the factors of the kinematic terms in sum (4), i.e. $(\mathbf{x}_i - \mathbf{x}_j)^{-1}$ and the potential term $e\mathbf{A}_i = \alpha r_i^{-1}$ (with $r_i = ||\mathbf{x}_i - \mathbf{x}_0||$), that suggests, both terms may have the same basic cause.

- Is it possible, to embed this theory into the framework of general relativity?

At last, it is to ask, of course, how far the theory is consistent with the current experimental knowledge. Especially, the representation of particle waves (DE BROGLIE-waves) and entangled quantum states would be a challenge.

A DIRAC-Equation in Matrix-Notation versus usual Spinor-Notation

As stated above, I will show here, that both notations are equivalent.
For this purpose, I start with the conventional representation for 4-spinors:[89]

$$i\gamma_\mu \partial^\mu \psi = m\psi. \tag{A.1}$$

There ψ is a 4-column vector, and the γ_μ are 4×4 matrices. Here, I use the WEYL-representation for the γ_μ:[90]

$$\gamma_0 = \begin{pmatrix} 0, -I_2 \\ -I_2, 0 \end{pmatrix}, \quad \text{and} \quad \gamma_k = \begin{pmatrix} 0, & \sigma_k \\ -\sigma_k, 0 \end{pmatrix}, \quad k = 1, 2, 3. \tag{A.2}$$

Then the 4-spinor is decomposable into two 2-spinors $\psi = \binom{\Psi}{\Phi}$, which transform independently, but different (see below) under LORENTZ-transformations, and (A.1) decomposes into a coupled system:

$$i(-\partial^0 + \sigma_k \partial^k)\Phi = m\Psi \quad \text{and} \quad i(-\partial^0 - \sigma_k \partial^k)\Psi = m\Phi. \tag{A.3}$$

Now I define a (HERMITEan) differential operator (a 2×2 matrix)[91]

$$\partial \stackrel{def}{=} \partial^0 - \sigma_k \partial^k \tag{A.4}$$

explicitly:

$$\partial = \begin{pmatrix} \frac{\partial}{\partial t} - \frac{\partial}{\partial z}, \frac{\partial}{\partial x} + i\frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} - i\frac{\partial}{\partial y}, \frac{\partial}{\partial t} + \frac{\partial}{\partial z} \end{pmatrix} = \frac{\partial}{\partial t} + \nabla. \tag{A.5}$$

Then the equations (A.3) read:

$$-i\partial\Phi = m\Psi \quad \text{and} \quad -i\bar{\partial}\Psi = m\Phi. \tag{A.6}$$

The LORENTZ-transformation T, $|T| = 1$ here operates as follows on the entities:

$$\partial \to T\partial T^\dagger, \quad \bar{\partial} \to \bar{T^\dagger}\bar{\partial}\bar{T}, \quad \Phi \to \bar{T^\dagger}\Phi, \quad \Psi \to T\Psi. \tag{A.7}$$

[89] see e.g. [4], pp. 24

[90] The 3 PAULI-matrices are again $\sigma_1 = \binom{0,1}{1,0}$, $\sigma_2 = \binom{0,-i}{i,\ 0}$, $\sigma_3 = \binom{1,\ 0}{0,-1}$

[91] note, that $\bar{I}_2 = I_2$ and $\bar{\sigma}_k = -\sigma_k$ holds, i.e. $\bar{\partial} = \partial^0 + \sigma_k \partial^k$ and all I_2, σ_k are HERMITEan matrices

Then both equations (A.6) are obviously covariant under this transformation. As usual, an electromagnetic interaction is introduced by the substitution $\partial^\mu \to \partial^\mu - ieA^\mu$, which gives here:

$$(i\partial + e\mathbf{A})\Phi = -m\Psi \quad \text{and} \quad (i\bar{\partial} + e\bar{\mathbf{A}})\Psi = -m\Phi. \tag{A.8}$$

Then the second equation of (A.8) is converted in the following manner.
One states the general formula for every 2x2 matrix M (M^T denoting transposed matrix): $\bar{M} = \sigma M^T \bar{\sigma}$, with $\sigma \stackrel{def}{=} i\sigma_2 = \left(\begin{smallmatrix} 0, & 1 \\ -1, & 0 \end{smallmatrix}\right)$.[92] Since (A.8b) has the form $\bar{M}\Psi = -m\Phi$, with $M = i\partial + e\mathbf{A}$, one gets $\sigma M^T \bar{\sigma}\Psi = -m\Phi$, which can be rewritten to [93] $M^T \sigma\Psi = -m\sigma\Phi$.

Of this one takes the complex conjugate, where $(M^T)^* = M^\dagger$:

$$M^\dagger \sigma\Psi^* = -m\sigma\Phi^*, \quad \text{with} \quad M^\dagger = -i\partial + e\mathbf{A}. \tag{A.9}$$

One then defines a new operator for 2-spinors $\underline{\widetilde{\Psi} \stackrel{def}{=} \sigma\Psi^*}$, which obeys $\widetilde{\widetilde{\Psi}} = -\Psi$ (since $\sigma^2 = -1$) and with that eq. (A.9) then writes $(-i\partial + e\mathbf{A})\widetilde{\Psi} = -m\widetilde{\Phi}$.
One then can combine both equations into one 2x2 matrix equation

$$e\mathbf{A}(\Phi, \widetilde{\Psi}) + i\partial(\Phi, -\widetilde{\Psi}) = -m(\Psi, \widetilde{\Phi}). \tag{A.10}$$

Now one defines the "spinor-matrix" $P \stackrel{def}{=} (\Phi, \widetilde{\Psi})$ and states $\overline{P^\dagger} = -(\Psi, \widetilde{\Phi})$, [94] and with the auxiliary matrix $S \stackrel{def}{=} \left(\begin{smallmatrix} i, & 0 \\ 0, & -i \end{smallmatrix}\right)$ finally gets:[95]

$$\underline{e\mathbf{A}P + \partial PS = m\overline{P^\dagger}}. \tag{A.11}$$

Note, that according to above definitions P transforms consistently with $P \to \overline{T}^\dagger P$ under LORENTZ-transformations and the equation $(A.11)$ is obviously covariant.

Gauge covariance is in this notation represented with the local transformation $P \to PU$, with $U \stackrel{def}{=} e^{\lambda S}$ (where $(\lambda(\mathbf{x})$ is a real, scalar function of space-time). Then holds (the parentheses are set here, to denote the action of the differential operator ∂): $\partial(PU) = (\partial P)U + (\partial\lambda)PUS$. Then, equation (A.11) is covariant, if the simultaneous transformation $e\mathbf{A} \to e\mathbf{A} + \partial\lambda$ is used.

---

[92] The reason is, that the bar-operation means spatial inversion $(x, y, z) \to (-x, -y, -z)$, and that is equal to the combined operation of transposing (i.e. $y \to -y$) and a rotation around y of 180°, given by $T = i\sigma_2$.

[93] trivially, since $\bar{\sigma} = -\sigma, \sigma^2 = -1$

[94] An explicit proof is $\Phi = \left(\begin{smallmatrix} \phi_1 \\ \phi_2 \end{smallmatrix}\right)$, $\Psi = \left(\begin{smallmatrix} \psi_1 \\ \psi_2 \end{smallmatrix}\right)$, $\widetilde{\Psi} = \left(\begin{smallmatrix} \psi_2^* \\ -\psi_1^* \end{smallmatrix}\right)$, $P = \left(\begin{smallmatrix} \phi_1, & \psi_2^* \\ \phi_2, & -\psi_1^* \end{smallmatrix}\right)$, $P^\dagger = \left(\begin{smallmatrix} \phi_1^*, & \phi_2^* \\ \psi_2, & -\psi_1 \end{smallmatrix}\right)$, $\overline{P^\dagger} = \left(\begin{smallmatrix} -\psi_1, & -\phi_2^* \\ -\psi_2, & \phi_1^* \end{smallmatrix}\right) = -(\psi, \widetilde{\phi})$.

[95] By using $S^2 = -1$ follows (e.g. by TAYLOR expansion): $e^{\lambda S} = \cos\lambda + S\sin\lambda = \left(\begin{smallmatrix} e^{i\lambda}, & 0 \\ 0, & e^{-i\lambda} \end{smallmatrix}\right)$.

The *stationary case* is given with the ansatz $P(\mathbf{r},t) = P_0(\mathbf{r})U(t)$, with $U(t) \stackrel{def}{=} e^{-\varepsilon t S}$, which (since $\partial_t P = -\varepsilon P S$)[96] results in:

$$(e\mathbf{A} + \varepsilon)P_0 + \nabla P_0 S = m\overline{P_0^\dagger}. \tag{A.12}$$

B Relativistic Electrodynamics in Matrix-Notation

I will shortly sketch here the basic equations of relativistic electrodynamics in matrix-notation without explicit proofs. Each equation can be checked, e.g. by converting it to usual component notation.

The tensor of the electromagnetic field is defined from the vector potential by:[97]

$$F \stackrel{def}{=} \frac{1}{2}(\bar{\partial}\mathbf{A} - \bar{\mathbf{A}}\partial). \tag{A.13}$$

It is a traceless matrix ($F + \overline{F} = 0$, by definition) and obeys the transformation rule $F \to \bar{T}^\dagger F T^\dagger$. It can be decomposed into a HERMITEan and anti-HERMITEan part, that are the electrical and magnetical field vectors, which both are HERMITEan, traceless matrices ($E^\dagger = E, \quad B^\dagger = B$):

$$F = E + iB \quad \text{and} \quad F^\dagger = E - iB. \tag{A.14}$$

Therefore, it is obvious, that both transform independently under spatial rotations, but are mixed under special LORENTZ-transformations.

The MAXWELL-equations are simply (with $\mathbf{J}$ as current, also HERMITEan)[98]

$$\mathbf{J} = \partial F, \tag{A.15}$$

and the equation of continuity (follows from last eq. with $F + \bar{F} = 0$) reads as

$$\mathcal{T}(\partial\overline{\mathbf{J}}) = \partial\overline{\mathbf{J}} + \mathbf{J}\overline{\partial} = 0. \tag{A.16}$$

Finally, the LORENTZ-force on a particle with mass m and electrical charge e, that is moving with the relativistic velocity vector $\mathbf{u} = d\mathbf{x}/d\tau$[99] results in an acceleration vector $\mathbf{a} = d\mathbf{u}/d\tau$:[100]

$$\underline{\mathbf{a} = \frac{e}{2m}(\mathbf{u}F + F^\dagger\mathbf{u}).} \tag{A.17}$$

[96] Since the scalar operator ∂_t commutes with P_0 and $\partial_t U = -\varepsilon U S$. Also obviously U commutes with S and $\overline{U^\dagger} = U$.

[97] Contrary to usual notations, here differential operators like ∂ can operate to the right, resp. left. In ambiguous cases, therefore the operand should be marked.

[98] these are actually 8 real equations, for the real and imaginary parts!

[99] τ is the eigentime, given from $d\tau = \sqrt{|d\mathbf{x}|}$

[100] The orthogonality of $\mathbf{a}, \mathbf{u}$ is written as $\mathcal{T}(\mathbf{a}\bar{\mathbf{u}}) = 0$ and follows directly from (A.17).

At last, I have to derive an identity for the last term of above equation, valid for arbitrary $\mathbf{u}$, which is used in the section 5:[101]

$$\begin{aligned}\mathbf{u}F + F^\dagger\mathbf{u} &= \frac{1}{2}(\mathbf{u}(\bar\partial\mathbf{A} - \bar{\mathbf{A}}\partial) + (\mathbf{A}\bar\partial - \partial\bar{\mathbf{A}})\mathbf{u}) \\ &= \frac{1}{2}(\mathbf{u}(\mathcal{T}(\bar\partial\mathbf{A}) - 2\bar{\mathbf{A}}\partial) + (2\mathbf{A}\bar\partial - \mathcal{T}(\partial\bar{\mathbf{A}}))\mathbf{u})) \\ &= \mathbf{A}\bar\partial\mathbf{u} - \mathbf{u}\bar{\mathbf{A}}\partial = \mathbf{A}\bar\partial\mathbf{u} + \underbrace{\mathbf{A}\bar{\mathbf{u}}\partial - \mathbf{A}\bar{\mathbf{u}}\partial}_{=0} - \mathbf{u}\bar{\mathbf{A}}\partial \\ &= \mathcal{T}(\bar\partial\mathbf{u})\mathbf{A} - \partial\mathcal{T}(\mathbf{A}\bar{\mathbf{u}}). \end{aligned} \tag{A.18}$$

C Differential Calculus and Approximations for Matrices

The formulas stated here are standard vector analysis, they are shortly listed here for readers, not so familiar with the notations in this paper.

The total differential for any field (matrix or scalar) U is given simply by

$$dU(\mathbf{x}+\mathbf{dx}) = U(\mathbf{x}+\mathbf{dx}) - U(\mathbf{x}) = \frac{1}{2}\mathcal{T}(\mathbf{dx}\bar\partial)U. \tag{A.19}$$

The simple explanation is, that the scalar invariant is explicitly written: $\frac{1}{2}\mathcal{T}(\mathbf{dx}\bar\partial) = dt\partial_t + dx\partial_x + \cdots$

One often above used approximation is for the expression $(X+\delta)^{-1}$, where X, δ are both matrices, with $|X| >> |\delta|$. However, the following approximation holds for any algebra. One states[102]

$$(X+\delta)^{-1} = (X(1+X^{-1}\delta))^{-1} = (1+X^{-1}\delta))^{-1}X^{-1} \approx (1-X^{-1}\delta))X^{-1} \tag{A.20}$$

D Matrix-Notation and Quaternions

Quaternions offer an elegant method for many computations, especially on the unit sphere and generally with space rotations.
They are representable by the sub-algebra of matrices, obeying $Q^\dagger = \overline{Q}$.[103]
The general form is obviously, with arbitrary complex α, β:

$$Q = \begin{pmatrix} \alpha, & \beta \\ -\beta^*, & \alpha^* \end{pmatrix}. \tag{A.21}$$

[101] Note, that $\mathcal{T}(\bar\partial\mathbf{A}) = \mathcal{T}(\partial\bar{\mathbf{A}})$.

[102] The expansion $(1-\delta)^{-1} = 1 + \delta + \delta^2 + \cdots$ can be easily checked by multiplying both sides with $(1-\delta)$. It converges, if $\lim_{n\to\infty}\delta^n = 0$, which is guaranteed by $|\delta| < 1$

[103] It is trivial, that any product of two quaternions is a quaternion again.

To represent a pure space vector $\mathbf{v}$ with quaternions, one uses $Q = i\mathbf{v}$, which is obviously a quaternion, since $\overline{\mathbf{v}} = -\mathbf{v}$.[104]
The quaternionic units $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ are consequently equal to $(i\sigma_1, i\sigma_2, i\sigma_3)$, giving (an arbitrary real s can be added, since it is not changed by rotations):

$$Q = \begin{pmatrix} s + iz, ix + y \\ ix - y, s - iz \end{pmatrix} = s + x\mathbf{i} + y\mathbf{j} + z\mathbf{k}. \tag{A.22}$$

The norm (here as matrix determinant) of a quaternion is always a positive real: $|Q| = |\alpha|^2 + |\beta|^2 = s^2 + x^2 + y^2 + z^2$.

Ordinary space rotations are directly represented by normalized quaternions, following from $T^\dagger = \overline{T}$ (i.e. also $TT^\dagger = T^\dagger T = 1$), and consequently the whole apparatus of the 3-dimensional vector space can be drawn with quaternions.

E.g. a rotation around any (space) axis $A = \mu_1\mathbf{i} + \mu_2\mathbf{j} + \mu_3\mathbf{k}$ (with $|A| = \sum \mu_i^2 = 1$) by an angle λ, is represented by the transformation matrix $T = e^{\lambda A} = \cos\lambda + A\sin\lambda$, which is obviously a normalized quaternion.

E Orthogonal Polynoms and LAGRANGE-Formalism

This chapter is intended to illuminate the general correspondencies between eigenvalue problems (represented by LAGRANGians) and orthogonal polynoms.[105]
In fact, this relationship was the motivation to engage in the above theory. It shows, that many problems of mathematical physics, described by eigenvalue problems, can be reduced to small sets of equations for the roots of corresponding orthogonal polynoms.

The pair of DIRAC radial equations for the 1-electron atom are used here, as especially related example, yet there exist many other applications.
All following refers to the one-dimensional case, however.[106] For more than one dimension, there will probably exist similar methods.

In the following, I will sketch some major relations for OP. Many of them (but not all), can be also found in standard textbooks, but derived with different formalisms.

E.1 Basic Formulas for OP

Definition: an OP of degree n : $P^{(n)}(x)$ is the (unique) polynom, associated

[104] MINKOWSKI matrices with time components, however, cannot be represented directly.
[105] Orthogonal polynoms are mainly used in numerical mathematics, e.g. to compute integrals. Their usefulness in problem solving is widely unknown, however.
[106] Thus all variables in this section are simple reals.

with an interval $[a, b]$ and a weight function $w(x) \geq 0, x \in [a, b]$, that is orthogonal to *all polynoms* $Q(x)$ of degree $q < n$, i.e.:[107]

$$\int_a^b dx w(x) P^{(n)}(x) Q(x) = 0. \tag{A.23}$$

These polynoms are unique up to a constant factor, of course. The roots, however, are unique. In the following we only deal with polynoms of the form $(x - x_1) \cdots (x - x_n)$, i.e. the highest coefficient is unity. These are called *monic polynoms*. With this condition they are unique.

It follows immediately, that two OP of different degrees n, m: $P^{(n)}, P^{(m)}$, are orthogonal (one is a polynom of lower degree).

In the following, the superscript of $P^{(n)}$ and the integral boundaries $[a, b]$ are omitted, however, since they are considered fixed.

Let $P(x) = \prod_{i=1}^{n} (x - x_i) = (x - x_1) \cdots (x - x_n)$, where all x_i are real and distinct.

Now one defines n associated *partial polynoms* to P, each of degree $n - 1$: $P_k(x) \stackrel{def}{=} \prod_{i \neq k}^{n} (x - x_i), \quad k = 1, \ldots, n$, see e.g. [7], pp. 502.[108]
Then by definition, P is also orthogonal to all P_k.
The partial polynoms P_i are also mutual orthogonal ($\int w P_1 P_2 = 0$). This is easy to see, if one expands e.g.[109] $P_1 P_2 = (\circ(x - x_2) \cdots)((x - x_1) \circ \cdots) = P(x - x_3) \cdots$.
Similarly follows $\int w \, x P_1 P_2 = 0$.

Additionally, one defines partial polynoms P_{kl} of second order (and similarly of higher order):

$$P_{kl} \stackrel{def}{=} \prod_{i \neq kl} (x - x_i), \quad P_{kl} = P_{lk}, \quad P_{kk} \stackrel{def}{=} 0. \tag{A.24}$$

With these definitions, I state some important equations, which can be easily proved with standard methods:

$$P_1 P_2 = P P_{12}, \qquad P_1 - P_2 = (x_1 - x_2) P_{12}, \tag{A.25}$$

[107] Thus, it roots can be computed e.g. with the following n equations: $\int dx w P^{(n)} = \int dx w P^{(n)} x = \int dx w P^{(n)} x^2 = \cdots = \int dx w P^{(n)} x^{n-1} = 0$.

[108] They are proportional to the LAGRANGE-polynoms, which are defined as $L_k = \prod_{i \neq k}^{n} ((x - x_i)/(x_k - x_i))$, i.e. $P_k(x) = \pi_k L_k(x)$, with $\pi_k = P_k(x_k) = \prod_{i \neq k}^{n} (x_k - x_i)$

[109] The $\circ$ mark stands here and sometimes in the following for omitted factors, to make the products more readable. Also, the subscripts $1, 2$ here denote arbitrary, but different indices from interval $1, \ldots, n$.

$$P' = P_1 + P_2 + \cdots, \qquad P'_1 = P_{12} + P_{13} + \cdots = \sum_{i\neq 1} \frac{P_1 - P_i}{x_1 - x_i}.$$

One now considers the *master integral*

$$\mathcal{I}(x_1, \cdots, x_n) \stackrel{def}{=} \int wP^2 = \int w(x-x_1)\cdots^2 (x-x_n)^2 > 0. \tag{A.26}$$

It is very easy to show, that this integral is *minimal* w.r.t all x_i:[110] At first it is stationary, since $\frac{\partial \mathcal{I}}{\partial x_i} = -2\int wPP_i = 0$. Secondly, it is a real minimum, since (here I define the n new constants $\rho_i \stackrel{def}{=} \int wP_i^2$)

$$\frac{\partial^2 \mathcal{I}}{\partial x_i^2} = 2\int wP_i^2 = 2\rho_i > 0 \quad \text{and} \quad \frac{\partial^2 \mathcal{I}}{\partial x_i x_j} = 0. \tag{A.27}$$

One can now (uniquely) expand an arbitrary polynom $f(x)$ of degree $\leq n-1$ by the partial polynoms P_i, with n constants f_i:

$$f(x) = \sum_i f_i P_i(x). \tag{A.28}$$

Then for two arbitrary polynoms f, g (of degree $\leq n-1$) and a linear function $\mu = a + bx$, easily follows (with $\mu_i \stackrel{def}{=} \mu(x_i)$):[111]

$$\int w\mu fg = \sum_i \rho_i \mu_i f_i g_i. \tag{A.29}$$

In fact, from this formula follows, that *every polynom* of degree $\leq 2n-1$ can be integrated *exactly* by its values at the n grid points x_i.

All OP also obey a linear, second order differential equation (with λ as eigenvalue):

$$uy'' + vy' + \lambda y = 0. \tag{A.30}$$

Here $u = u_0 + u_1 x + u_2 x^2$ is a polynom of degree ≤ 2, which must not have any zeros in the interval $[a, b]$ and $v = v_0 + v_1 x$ is linear.[112]

If then the ansatz $y = P(x) = (x-x_1)\cdots(x-x_n)$ is made and $\lambda \neq 0$, at the zeros obviously must hold $[uy'' + vy']_{x=x_k} = 0$. With $y'(x_k) = P_k(x_k)$ and $y''(x_k) = 2P_k(x_k)\sum_{i\neq k} \frac{1}{x_k - x_i}$ results a system of equations for the zeros:

$$2\sum_{i\neq k} \frac{1}{x_k - x_i} + \frac{v(x_k)}{u(x_k)} = 0. \tag{A.31}$$

[110] It is then minimal among all monic polynoms.

[111] This formula is widely used for numerical integrations, however the determination of the coefficients ρ_i is often quite complicated. In the following, I will show a much more simple way to compute them, which I have not yet found in the literature.

[112] By this representation, all OP systems can be easily classified. Some important examples are: LEGENDRE-, TSCHEBYSCHEFF-, JACOBI-, LAGUERRE- and HERMITE-polynoms.

The proof, that the polynom $P = (x - x_1) \cdots (x - x_n)$ then fulfills equation (A.30) is quite simple: Since $uP'' + vP'$ is a polynom of degree $\leq n$, and has (following above relations) zeros at all x_k and therefore must be proportional to P.[113]
This set of equations uniquely determines the set of zeros, and also can be used to set up numerical methods to compute them.

It also can be shown easily, that the weighting function $w(x)$ is then related to the pair u, v by $(wu)' = wv$, i.e. $w = \frac{1}{u} e^{\int \frac{v}{u}\, dx}$.

E.2 Weight Factors for OP-Integrals

As last prerequisite, a general, explicit formula for the weighting constants ρ_i is needed (which I did not found in any textbooks). To get it, I start with the expression (again with $u_i \stackrel{def}{=} u(x_i)$):[114]

$$\Delta_{12} = \int wuP_{12}P' = \frac{1}{x_2 - x_1} \int wu(P_1^2 - P_2^2) = u_1\rho_1 - u_2\rho_2. \tag{A.32}$$

On the other hand, by partial integration, one easily shows, that $\Delta_{12} = 0$, consequently with some constant k, follows:[115]

$$\underline{u_1\rho_1 = u_2\rho_2 = \cdots = k = const.} \tag{A.33}$$

E.3 Solving the Radial DIRAC-Equations with OP

With the help of above relations, the extremal principles can be investigated. Here I consider, what one may call "dual eigenvalue" problems, e.g. of the type of the pair of radial DIRAC equations, where there are two functions to variate independently[116] (the name of the variable x is changed from here on to r and the intervall to use, is of course, $r \in [0, \infty]$). The LAGRANGian here has the general form (where a, b, c are some fixed functions of r).[117]

$$\mathcal{L}(f, g) = \int_0^\infty dr(f'g - g'f + 2afg + bf^2 + cg^2) \to extr. \tag{A.34}$$

For the DIRAC equation one has to use $a = -\frac{\kappa}{r},\ b = \varepsilon + \frac{\alpha}{r} - m,\ c = \varepsilon + \frac{\alpha}{r} + m$, see e.g. [8].

[113] The eigenvalue can be easily computed from the coefficients of x^n: $\lambda_n = -n(n-1)u_2 - nv_1$.
[114] which holds for any polynom $u(x)$ of degree ≤ 2
[115] The value of k can be computed by evaluating the integral $\int wuP'^2$, then follows $k = -(v_0 + (2n-1)v_1)\mathcal{I}$, where v_0, v_1 are the coefficients of $v = v_0 + v_1 x$.
[116] Also LAGRANGians of ordinary, second order differential equations can be represented in this form. Consider for example the simple integral $\mathcal{L}(y) = \int (y')^2 + ay^2 \to extr.$, which leads to $y'' = ay$. The last eq. is equivalent to the first order pair $y' = u, u' = ay$, which in turn is represented by the LAGRANGian $\mathcal{L}(y, u) = \int yu' - uy' - ay^2 + u^2$.
[117] With standard variational methods, using $\int (f'g + g'f) = [fg]_0^\infty = 0$, one easily proves, that it is equivalent to the pair of first order DGL: $f' + af + cg = 0$ and $g' - ag - bf = 0$.

Now the polynomial ansatz is made, with a common factor $\varphi(r)$: $f = \varphi F$, $g = \varphi G$, where F, G shall be polynoms of degree $n-1$ (it is presumed to be possible, here), resulting in:[118]

$$\mathcal{L}(F,G,\varphi) = \int_0^\infty dr\varphi^2(F'G - G'F + 2aFG + bF^2 + cG^2) \to extr. \quad \text{(A.35)}$$

Since ra, rb, rc are linear expressions of r, one uses the weighting function $w(r) = \varphi^2/r$, so the factor in the integrand becomes a polynom of degree $2(n-1)+1 = 2n-1$, and the above apparatus can be applied:

$$\mathcal{L} = \int_0^\infty drw[r(F'G - G'F + 2aFG + bF^2 + cG^2)]. \quad \text{(A.36)}$$

The polynoms F, G then are represented as $F(r) = \sum_1^n f_i P_i$, $G(r) = \sum_1^n g_i P_i$, with $2n$ constants f_i, g_i. One now uses for the derivations F', G' the formula:

$$F' = \sum_i \hat{f}_i P_i, \quad \text{with} \quad \hat{f}_i \stackrel{def}{=} \sum_{j\neq i} \frac{f_i + f_j}{r_i - r_j}. \quad \text{(A.37)}$$

Inserting this all in eq. (A.36), leads to a double sum:

$$\mathcal{L} = \int_0^\infty drw \sum_{ij} [r(\hat{f}_i g_j - \hat{g}_i f_j + 2af_i g_j + bf_i f_j + cg_i g_j)P_i P_j]. \quad \text{(A.38)}$$

If now the previously free variables $\{r_i\}$ are set to the zeros of the OP for the weighting function $w = \varphi^2/r$, then all integrals can be computed, and the expression becomes a simple sum (again defining $a_i = a(r_i), ...$):

$$\mathcal{L} = \sum_i \rho_i r_i (\hat{f}_i g_i - \hat{g}_i f_i + 2a_i f_i g_i + b_i f_i^2 + c_i g_i^2). \quad \text{(A.39)}$$

It can be shown, that the OP to use here, are LAGUERRE-polynoms, i.e. they belong to a weight function $w(r) = e^{-2\lambda r} r^{2\gamma-1}$, where $\lambda \stackrel{def}{=} \sqrt{m^2 - \varepsilon^2}$ and $\gamma \stackrel{def}{=} \sqrt{\kappa^2 - \alpha^2}$.[119] For these, one has $u(r) = r$, so from eq. (A.33) follows $\rho_i r_i = const. \stackrel{def}{=} k$ and I finally get the formula:

$$\underline{\mathcal{L} = k(\sum_{i\neq j} \frac{f_i g_j - g_i f_j}{r_j - r_i} + \sum_i (2a_i f_i g_i + b_i f_i^2 + c_i g_i^2)).} \quad \text{(A.40)}$$

This is exactly (except the constant factor k) the same as (38), q.e.d.

Again, the similarity to the starting point (A.34) is remarkable, however, a general discussion of the preconditions for this, should be left to interested mathematicians.

[118] The derivations of φ cancel out.

[119] The ansatz-factor function $\varphi(r)$ is then $\varphi = e^{-\lambda r} r^\gamma$.

F LAGRANGIAN for the Unit Sphere

Here I will shortly derive the discretization scheme for the unit sphere, that leads to the above discussed solutions of DIRAC equation for the atom, in section 4.3.[120]

The LAGRANGian for the angular part ($\mathbf{p}_i$ are the points on the unit sphere), that was derived there, is (see (36)):

$$\mathcal{L} = \sum_{ij} \mathcal{T}(\bar{A}_i \mathbf{p}_i (\mathbf{p}_i - \mathbf{p}_j)^{-1} A_j) - 2\kappa \sum_i |A_i|, \tag{A.41}$$

where the A_i are quaternionic matrices ($\bar{A}_i = A_i^\dagger$), attached to the points and the double sum is to build over all edges $(\mathbf{p}_i, \mathbf{p}_j)$.

As shown below, the described grid, together with A_i is *stationary*, i.e. it makes the LAGRANGian , considered as function $\mathcal{L}(\mathbf{p}_i, A_i)$ extremal.

Any point on the unit sphere (x, y, z), $x^2 + y^2 + z^2 = 1$ is represented with spherical coordinates ϑ, φ by the matrix

$$\mathbf{p} = \begin{pmatrix} z, & x - iy \\ x + iy, & -z \end{pmatrix} = \begin{pmatrix} \cos\vartheta, & \sin\vartheta e^{-i\varphi} \\ \sin\vartheta e^{i\varphi}, & -\cos\vartheta \end{pmatrix}.$$

Now one introduces the conformal one-to-one mapping of the sphere to the complex plane[121] $\chi \in \mathbf{C}$ with:[122]

$$\chi = \tan\frac{\vartheta}{2} e^{i\varphi} = \frac{\sin\vartheta e^{i\varphi}}{1 + \cos\vartheta}. \tag{A.42}$$

Then one gets with simple trigonometric identities: $z = \cos\vartheta = \frac{1-|\chi|^2}{1+|\chi|^2}$ and $x + iy = \sin\vartheta e^{i\varphi} = \frac{2\chi}{1+|\chi|^2}$, consequently:

$$\mathbf{p} = \frac{1}{1 + |\chi|^2} \begin{pmatrix} 1 - |\chi|^2, & 2\chi^* \\ 2\chi, & |\chi|^2 - 1 \end{pmatrix}.$$

This matrix can be decomposed with the help of *spinor-matrix factors*[123] $Q = Q(\chi)$, which I define here as:

$$Q(\chi) \stackrel{def}{=} \begin{pmatrix} 1, & \chi^* \\ \chi, & -1 \end{pmatrix} \tag{A.43}$$

[120] Of course, also a more concise quaternionic representation of the following is feasible. However, since probably most readers are not very familiar with this formalism, I prefer the matrix notation here.

[121] This map is the inverse of the usual "RIEMANN sphere" map. Please note, that the complex number χ then transforms *linear fractionally* under ordinary space-rotations, namely if $T = \begin{pmatrix} \alpha, & \beta \\ -\beta^*, & \alpha^* \end{pmatrix}$ is a rotation (with $|T| = 1$), then follows $\chi \to \frac{\alpha\chi+\beta}{-\beta^*\chi+\alpha^*}$.

[122] E.g. the north pole $(0, 0, 1)$ is mapped to the origin of the complex plane $\chi = 0$, the south pole $(0, 0, -1)$ to the infinite point $\chi = \infty$ and the equator to the circle $|\chi| = 1$.

[123] These factors transform similar to spinors under rotations, not MINKOWSKI space vectors!

and the constant matrix $U \stackrel{def}{=} \left(\begin{smallmatrix}1, & 0\\ 0, & -1\end{smallmatrix}\right)$, namely as:[124]

$$\mathbf{p} = QUQ^{-1}. \tag{A.44}$$

With the help of this decomposition formula it is easy to express the required difference vector of *two arbitrary points* $\mathbf{p}_1, \mathbf{p}_2$ on the unit sphere (the inverse of this difference is the crucial part in computing the LAGRANGian sum in (A.41)) and $Q_i \stackrel{def}{=} Q(\chi_i)$:[125]

$$\mathbf{p}_1 - \mathbf{p}_2 = Q_1 U Q_1^{-1} - Q_2 U Q_2^{-1} = Q_2^{-1} \underbrace{(Q_2 Q_1 U - U Q_2 Q_1)}_{\stackrel{def}{=} D_{21}} Q_1^{-1} \tag{A.45}$$

With $V_{21} \stackrel{def}{=} Q_2 Q_1 = \left(\begin{smallmatrix}1+\chi_2^*\chi_1, & \chi_1^* - \chi_2^*\\ \chi_2 - \chi_1, & 1+\chi_2\chi_1^*\end{smallmatrix}\right)$ it is to see, that the difference in the brackets of this expression D_{21}, is the anticommuting part of the factors U and V_{21} and can easily be computed as:

$$D_{21} = 2\begin{pmatrix}0, & \chi_2^* - \chi_1^*\\ \chi_2 - \chi_1, & 0\end{pmatrix}.$$

With this equation (A.45) is easily invertable and one finally gets:

$$\mathbf{p}_1(\mathbf{p}_1 - \mathbf{p}_2)^{-1} = Q_1 U Q_1^{-1} Q_1 D_{21}^{-1} Q_2 = \frac{1}{2} Q_1 \begin{pmatrix}0, & \frac{1}{\chi_2 - \chi_1}\\ -\frac{1}{\chi_2^* - \chi_1^*}, & 0\end{pmatrix} Q_2. \tag{A.46}$$

Now one makes the following substitution for the A_i, to simplify the double sum in (A.41), with the complex constants μ_i, ν_i:[126]

$$A_i = Q_i^{-1}\begin{pmatrix}\mu_i^*, & \nu_i\\ \nu_i^*, & -\mu_i\end{pmatrix}. \tag{A.47}$$

Then follows $|A_i| = \frac{1}{|Q_i|}(-\mu_i\mu_i^* - \nu_i\nu_i^*) = \frac{|\mu_i|^2 + |\nu_i|^2}{1+|\chi_i|^2}$.
The LAGRANGian in (A.41) then simplifies to (it is obviously real as required):

$$\mathcal{L}(\mu_i, \nu_i, \chi_i) = \sum_{ij}\left(\frac{\nu_j^*\mu_i}{\chi_j - \chi_i} + \frac{\nu_j\mu_i^*}{\chi_j^* - \chi_i^*}\right) - 2\kappa\sum_i \frac{|\mu_i|^2 + |\nu_i|^2}{1+|\chi_i|^2}. \tag{A.48}$$

As always, one has to find *stationary points* in parameter space, which is here $\{\mu_i, \nu_i, \chi_i\}, i = 1, \ldots, n$.

Since all parameters are simple scalars, this can be done by setting the partial derivations zero, which gives $3n$ equations, $k = 1, \ldots n$:[127]

$$\frac{\partial\mathcal{L}}{\partial\mu_k} = \frac{\partial\mathcal{L}}{\partial\nu_k} = \frac{\partial\mathcal{L}}{\partial\chi_k} = 0$$

[124] For an explicit proof consider $|Q| = -(1+|\chi|^2)$, $Q^2 = 1 + |\chi|^2$ and $Q^{-1} = \frac{1}{1+|\chi|^2}Q$

[125] Consider from above $Q_k^{-1} U Q_k = Q_k U Q_k^{-1}$

[126] This is the most general ansatz, if the quaternionic restriction $\bar{A}_i = A_i^\dagger$ is considered.

[127] Us usual the complex conjugate of any parameter can be considered as independent, and since the expression $\mathcal{L}$ is real, the derivation by it leads to an equivalent equation.

Namely, (by the variations of ν_i^*, μ_i^*) result the first $2n$ equations (for $k = 1, \ldots, n$):[128]

$$\sum_i \frac{\mu_i}{\chi_k - \chi_i} \stackrel{!}{=} 2\kappa \frac{\nu_k}{1+|\chi_k|^2} \quad \text{and} \quad \sum_i \frac{\nu_i}{\chi_k^* - \chi_i^*} \stackrel{!}{=} -2\kappa \frac{\mu_k}{1+|\chi_k|^2}. \tag{A.49}$$

The variation of all χ_k leads to the equations ($k = 1, \ldots, n$):[129]

$$-\sum_i \frac{\nu_k^*\mu_i - \nu_i^*\mu_k}{(\chi_k - \chi_i)^2} + 2\kappa \frac{(|\mu_k|^2 + |\nu_k|^2)\chi_k^*}{(1+|\chi_k|^2)^2} = 0. \tag{A.50}$$

Now I will show, that the point in parameter space, given by the simple formulas $\underline{\mu_i = c}$, $\underline{\nu_i = c\chi_i^*}$ with real constant c[130] and any set of points $\{\chi_k\}$ (on the unit sphere by definition), that obeys

$$\sum_i \frac{1 + \chi_i\chi_k^*}{\chi_k - \chi_i} \stackrel{!}{=} 0, \quad k = 1, \ldots, n \tag{A.51}$$

fulfills all $3n$ conditions above. Like all others, the above sum is *not to build over all* $i \neq k$, but only over the edges (χ_i, χ_k), which are presented in the following.[131] This grid of points χ_k can, as to expect, be derived from *spherical harmonics* (this is described below).

Simple rearrangement gives two equivalent sets of equations, wherein l is the number of summands (edges i, k), which should be equal for all χ_k, $k = 1, \ldots, n$:

$$\sum_i \frac{1}{\chi_k - \chi_i} = l\frac{\chi_k^*}{1+|\chi_k|^2} \quad \text{and} \quad \sum_i \frac{\chi_i}{\chi_k - \chi_i} = -l\frac{1}{1+|\chi_k|^2}. \tag{A.52}$$

Then all $3n$ conditions (A.49, A.50) are fulfilled, i.e. **the stationarity of** $\mathcal{L}(\mu_i, \nu_i, \chi_i)$ **is proven**, if the eigenvalue κ is set to $\underline{\kappa = \frac{l}{2}}$, q.e.d.[132]

A second stationary point is obviously given with the same set of χ_k, but[133]

$$\mu_i = c\chi_i, \quad \nu_i = c, \quad \kappa = -\frac{l}{2}.$$

Please note, that both cases $\kappa = \pm\frac{l}{2}$ describe *different quantum states* in the DIRAC equation (see e.g. [8], pp. 119).

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[128] Consider the complex differentiation rules, e.g. $\frac{\partial|\chi|^2}{\partial\chi} = \frac{\partial(\chi\chi^*)}{\partial\chi} = \chi^*$.

[129] The double sum contains each pair i, k *twice*.

[130] The resulting matrix is then simply $A_i = Q_i^{-1} c Q_i = cI$.

[131] These equations are indeed *covariant* under space rotations, described here as linear fractional transformation of all χ_i, like mentioned above.

The simplest possible example set is given with $n = 2$, i.e. two points χ_1, χ_2 with one edge between them. Both (A.51), for $k = 1, 2$, then simply require $1 + \chi_1\chi_2^* \stackrel{!}{=} 0$. This condition says, that the two points must be *antipodes* on the sphere, while one of them, e.g. χ_1, is freely variable.

[132] which is to see by simply inserting the above ansatz: $\mu_i = 1, \nu_i = \chi_i^*$ and (A.52).

[133] The resulting matrix is then $A_k = Q_k^{-1} c \begin{pmatrix} \chi_k^*, 1 \\ 1, -\chi_k \end{pmatrix} = \frac{c}{1+|\chi_k|^2} \begin{pmatrix} 2\chi_k^*, 1-|\chi_k|^2 \\ |\chi_k|^2 - 1, 2\chi_k \end{pmatrix} = c \begin{pmatrix} x_k - iy_k, z_k \\ -z_k, x + iy_k \end{pmatrix}$

Finally I will shortly sketch, how a set of $\{\chi_k\}$ and the assigned edges, that fulfill (A.51), can be constructed using *spherical harmonics*.
There might exist also other grids, which give the same result, but I was not able to find anyone.

The nodes are supposed to be arranged on h latitude circles (which are defined here by $|\chi| = const.$), in the way that on every circle are $2m$ equidistant nodes.
I.e. one has $n = 2m \times h$ nodes and they can be assigned as (with real $t_k > 0$):

$$\chi = t_k e^{\pi i \frac{j}{m}}, \quad k = 1, \dots h, \quad j = 1, \dots 2m. \tag{A.53}$$

Edges shall be only on latitude circles (denoted as $i \in B(k)$) and longitude circles (as $i \in A(k)$):

$$\sum_i \frac{1}{\chi_k - \chi_i} = \sum_{i \in B(k)} \frac{1}{\chi_k - \chi_i} + \sum_{i \in A(k)} \frac{1}{\chi_k - \chi_i}. \tag{A.54}$$

This gives a total number of $l = 2m - 1 + 2h - 1 = 2(m + h - 1)$ edges connected to every node, since on each longitude circle j are actually $2h$ nodes: $t_k e^{\pi i \frac{j}{m}}$ and $t_k e^{\pi i \frac{j+m}{m}} = -t_k e^{\pi i \frac{j}{m}}$, $k = 1, \dots h$. This also means, that the opposite point of χ_k on the latitude circle, which is $-\chi_k$, counts *twice* in the sum (on both circles).

The summation on a latitude circle gives:[134]

$$\sum_{i \in B(k)} \frac{1}{\chi_k - \chi_i} = \frac{2m - 1}{2\chi_k}. \tag{A.55}$$

The summation on the longitude circle gives (the opposite point of χ_k on this circle, gives the summand $1/2\chi_k$):

$$\sum_{i \in A(k)} \frac{1}{\chi_k - \chi_i} = \frac{1}{2\chi_k} + \frac{t_k}{\chi_k} \left[\sum_{i \neq k} \left(\frac{1}{t_k - t_i} + \frac{1}{t_k + t_i} \right) \right]. \tag{A.56}$$

Consequently the complete sum over all edges becomes:

$$\sum_i \frac{1}{\chi_k - \chi_i} = \frac{\chi_k^*}{t_k^2} \Big[m + \sum_{i \neq k} \frac{2t_k^2}{t_k^2 - t_i^2} \Big]. \tag{A.57}$$

To prove corespondence to zeros of spherical harmonics, one subtitutes back to the cartesian coordinates, which is given by $t^2 = |\chi|^2 = \frac{1-z}{1+z}$. Then (A.57) can be expressed as

$$\sum_i \frac{1}{\chi_k - \chi_i} = \chi_k^* (1 + z_k) \Big[\frac{m}{1 - z_k} + \sum_i \frac{1 + z_i}{z_i - z_k} \Big].$$

[134] This formula can be proved using a general relation for the complex roots of $z^n = 1$, which are $z_k = e^{2\pi i k/n}$, $k = 1, \dots, n$, namely: $\sum_{k=1}^{n-1} \frac{1}{1-z_i} = \frac{n-1}{2}$, which again follows from $\frac{1}{1-z} + \frac{1}{1-1/z} = 1$.

The r.h.s. of this equation is then equal to the required expression

$$l\frac{\chi_k^*}{1+|\chi_k|^2} = l\chi_k^*\frac{1+z_k}{2} = (m+h-1)\chi_k^*(1+z_k)$$

to obey the stationarity conditions (A.52), if for all z_k holds:

$$\sum_i \frac{1}{z_k - z_i} = m\frac{z_k}{1-z_k^2}. \tag{A.58}$$

It is now easy to check, that (A.58) is fulfilled for the zeros of LEGENDRE functions of order $m + h$, namely $P_{m+h}^{m-1}(z)$ (see e.g. [3], pp. 282), with the methods of orthogonal polynoms presented here (see section E, eq. (A.31)).

As a summary of this chapter, I want to state, that all classical stationary states of the DIRAC equation are reproduced exactly above. However, it is not yet clear, by which principle some grids (e.g. with an odd number of nodes on a latitude circle) are suppressed.

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