A Flow Equation Approach Striving towards an Energy-Separating Hamiltonian Unitary Equivalent to the Dirac Hamiltonian with Coupling to Electromagnetic Fields

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Abstract

The Dirac Hamiltonian $H^{(D)}$ for relativistic charged fermions minimally coupled to (possibly time-dependent) electromagnetic fields is transformed with a purpose-built flow equation method, so that the result of that transformation is unitary equivalent to $H^{(D)}$ and granted to strive towards a limiting value $H^{(NW)}$ commuting with the Dirac $\beta$-matrix. Upon expansion of $H^{(NW)}$ to order $\frac{v^2}{c^2}$ the nonrelativistic Hamiltonian $H^{(SP)}$ of Schrödinger-Pauli quantum mechanics emerges as the leading order term adding to the rest energy $mc^2$. All the relativistic corrections to $H^{(SP)}$ are explicitly taken into account in the guise of a Magnus type series expansion, the series coefficients generated to order $\left(\frac{v^2}{c^2}\right)^n$ for $n \geq 2$ comprising partial sums of iterated commutators only. In the special case of static fields the equivalence of the flow equation method with the well known energy-separating unitary transformation of Eriksen is established on the basis of an exact solution of a reverse flow equation transforming the $\beta$-matrix into the energy-sign operator associated with $H^{(D)}$. That way the identity $H^{(NW)} = \beta \sqrt{H^{(NW)}H^{(NW)}}$ is established implying $H^{(NW)}$ being determined unambiguously. In contrast to $H^{(D)}$ its unitary equivalent $H^{(NW)}$ generates the motion of electrons and positrons in the presence of weak external fields now as entirely separated wave packets carrying mass $m$, charge $\pm |e|$ and spin $\pm \frac{\hbar}{2}$ respectively, yet those wave packets being by construction bare of any "Zitterbewegung", akin to classical particles moving along individual trajectories under the influence of the Lorentz force. Upon expansion of $H^{(NW)}$ to order $\left(\frac{v^2}{c^2}\right)^n$ for $n = 1, 2, 3, ...$ our results agree with results obtained recently by Silenko with a correction scheme developed for the original step-by-step FW-transformation method, the latter long-since known for not generating unambiguously a unitary equivalent Hamiltonian being energy-separating.

INTRODUCTION

Based on insight into the fundamental meaning of locality obtained by Newton and Wigner (NW) in 1949 for (freely moving) relativistic fermions [1], Foldy and Wouthuysen (FW) established in 1950 with their unitary transformation of the free Dirac Hamiltonian an interpretation of concepts like position or velocity or spin or orbital angular momentum [2], void of the well known paradoxical properties of operators in the Dirac representation

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(for instance the velocity operator having eigenvalues ±c) and thus agreeable to the physical intuition ascribed to a moving single particle.

For this reason we suggest to refer in the ensuing to the result H\(^{(NW)}\) of such a unitary transformation of the Dirac Hamiltonian H\(^{(D)}\) as the NW-Hamiltonian even if in H\(^{(D)}\) additional couplings to weak and slowly varying, possibly time-dependent electromagnetic fields are taken into account.

For a relativistic charged fermion with minimal coupling to a magnetostatic field a generalization of the unitary FW-transformation in closed form has been discovered by Case and also, along a different line of reasoning, by Eriksen, whose unitary transformation indeed applies as well to electrostatic and/or magnetostatic fields superposed.

In the ensuing a purpose-built flow equation approach is introduced resulting in a limiting value H\(^{(NW)}\) equivalent to a unitary transformation of the Dirac-Hamiltonian for a charged fermion with coupling to time-dependent electromagnetic fields, that in the special case of static fields turns out to be equivalent to the unambiguous energy-separating result obtained with the Eriksen transformation. The advantage of the new flow equation approach being that it provides in a lucid manner the expansion of H\(^{(NW)}\) in powers of v/c to arbitrary order, and that in the special case of static fields that expansion is in full agreement with corresponding results obtained by the (arduous) expansion of Eriksen’s transformation.

I. THE FLOW EQUATION METHOD

The so-called Hamiltonian flow equation method, originally developed by Wegner for problems in nonrelativistic many body physics, pertains to a continuous unitary transformation of a given Hamiltonian H via

\[
H(s) = U(s) H U^\dagger(s)
\]

\[
\frac{d}{ds} U(s) = \eta(s) U(s)
\]

\[
U(0) = 1_{4\times4}
\]

\[
\eta^\dagger(s) = -\eta(s)
\]
Given an antisymmetric generator \( \eta (s) \) for the flow, the unitary transformation of an hermitean operator \( H \) is determined solving an initial value problem

\[
\frac{d}{ds} H (s) = [\eta (s), H (s)]
\]

\( H (0) = H \)  \( (2) \)

Of course, the crux of the method is the choice of the generator \( \eta (s) \), with the essential point being, that \( \eta (s) \) controls the properties of the limiting value \( H (\infty) \). A comprehensive review discussing various generators with a multitude of applications of the Wegner flow equation method in nonrelativistic many body physics has been given by Kehrein [8]. Let us choose a most simple generator that depends on a constant hermitean operator \( \Gamma \) and consider a positive semi-definite functional as introduced by Brockett [9],[10]

\[
\Phi (s) \equiv \frac{1}{2} \text{tr} \left( (H (s) - \Gamma)^2 \right) \geq 0 \quad (3)
\]

Here \( H (s) \) is the solution of a flow with generator \( \eta (s) \), specified in terms of \( \Gamma \) as

\[
\eta (s) = [\Gamma, H (s)]
\]

\[
\frac{d}{ds} H (s) = [\eta (s), H (s)]
\]

\( H (0) = H \)  \( (4) \)

Exploiting the cyclic invariance of the trace one readily finds after a sequence of elementary adjustments

\[
\frac{d}{ds} \Phi (s) = \text{tr} \left[ (H (s) - \Gamma) \frac{d}{ds} H (s) \right]
\]

\[
= \text{tr} \left[ (H (s) - \Gamma) [\eta (s), H (s)] \right]
\]

\[
= \text{tr} \left[ (H (s) - \Gamma) [[\Gamma, H (s)], H (s)] \right]
\]

\[
= -\text{tr} \left[ [[H (s), \Gamma] [\Gamma, H (s)]] \right]
\]

\[
= -\text{tr} \left[ \eta^\dagger (s) \eta (s) \right]
\]

\[
\leq 0
\]

Because \( \Phi (s) \geq 0 \) for all \( s \geq 0 \) the only possible conclusion being that

\[
\lim_{s \to \infty} \frac{d}{ds} \Phi (s) = 0
\]

\( (6) \), i.e.

\[
\lim_{s \to \infty} \eta (s) = [\Gamma, H (\infty)] = 0_{4 \times 4}
\]

\( (7) \)
So, a double bracket flow of the type \([\mathbb{H}]\) indeed strives to a limiting value \(H(\infty)\) that commutes with the given hermitean operator \(\Gamma\).

A while ago Bylev and Pirner (BP) \cite{11} suggested a flow equation approach to obtain a unitary transformation of the Hamiltonian \(H^{(D)}\) for a Dirac particle moving in an external static electromagnetic potential, choosing as a generator

\[
\eta(s) = [\beta, H(s)]
\]  \hspace{1cm} (8)

and choosing as initial data at \(s=0\)

\[
H(0) = H^{(D)}
\]  \hspace{1cm} (9)

The afore propounded argument in the special case \(\Gamma = \beta\) at once reveals the limiting value \(H(\infty)\) of that flow being even, i.e.

\[
0_{4 \times 4} = \eta(\infty) = \beta H(\infty) - H(\infty) \beta
\]  \hspace{1cm} (10)

Actually, the result \(H(\infty)\) being an even operator was obtained in \cite{11} merely for a special case of perturbation theory, akin (but not identical) with the outcome of the perturbative procedure of consecutive step by step canonical transformations aiming at eliminating the odd terms in the Dirac Hamiltonian due to Foldy and Wouthuysen (FW) \cite{2}. Comparing the results obtained with the BP-method with the ones obtained by the FW-method a discrepancy arises in the 6\(^{th}\)-order of perturbation theory expanding in the small parameter \(\kappa = \frac{v}{c} \) \cite{12}. Mind because of the ambiguity in the definition of the sequence of operators with such a step-by-step method, a blockdiagonal operator resulting from several successive unitary \(4 \times 4\)-transformations is only guaranteed to give results being equivalent up to a \(2 \times 2\)-blockdiagonal unitary transformation, as earlier on was already emphasized by Pursey \cite{13} and by Eriksen and Kolsrud \cite{14}. However, as has been concisely discussed in an elucidating article by Costella and McKellar \cite{3}, the crucial finding of Foldy and Wouthuysen is not so much concerned with the (certainly useful) perturbative step by step elimination of the odd terms in a (possibly time-dependent) Dirac Hamiltonian, but is in the main concerned with the unravelling of a problem of interpretation with the four-component amplitude \(\Psi^{(D)}_{\mu}(r, t)\) that solves the Dirac equation.
II. A PROBLEM OF INTERPRETATION WITH THE FOUR-COMPONENT
DIRAC AMPLITUDE

In relativistic quantum mechanics a fermion with attributes mass \( m \), spin \( \pm \hbar \) and charge \( q_e = -|e| \), say moving in the presence of electrostatic and magnetostatic fields, is described in terms of a four-component amplitude \( \Psi_{\mu}^{(D)}(\mathbf{r}, t) \) solving the Dirac equation [15] :

\[
i\hbar \partial_t \Psi_{\mu}^{(D)}(\mathbf{r}, t) = \mathbf{H}_{\mu,\mu'}^{(D)} \Psi_{\mu'}^{(D)}(\mathbf{r}, t)
\]

\( \mu, \mu' \in \{1, 2, 3, 4\} \)

Here

\[
\mathbf{H}^{(D)} = mc^2 \beta + c\alpha_b \Pi_b + q_e \Phi(x)
\]

denotes the relativistic Hamiltonian of the fermion with minimal coupling to electromagnetic fields in Dirac-Pauli representation, with the well known \( 4 \times 4 \) matrices \( \beta \) and \( \alpha_b \) anticommuting and being of square equal to unity, see for instance [16], [17], [18], [19]. The magnetic induction field \( \mathbf{B} = \text{rot} \mathbf{A} \) is encoded in the gauge invariant derivative operator composed of the Cartesian components of the conjugate momentum and position operators, \( p_b \) and \( x_a \), of fundamental quantum mechanics

\[
\Pi_b(p, x) \equiv P_b = p_b - q_e A_b(x)
\]

\[ [p_b, x_a] = \frac{\hbar}{i} \delta_{a,b} \mathbf{1} \]

According to the superposition principle the Dirac amplitude \( \Psi_{\mu}^{(D)}(\mathbf{r}, t) \) may be represented as a linear combination of a complete system of orthonormal four-component eigenfunctions \( U_{\mu}^{(D)}(\mathbf{r}, k) \) and \( V_{\mu}^{(D)}(\mathbf{r}, \tilde{k}) \) of \( \mathbf{H}^{(D)} \), entailing both, the positive and the negative energy eigenvalues \( E_k > 0 \) and \( -E_{\tilde{k}} < 0 \) :

\[
\Psi_{\mu}^{(D)}(\mathbf{r}, t) = \sum_k U_{\mu}^{(D)}(\mathbf{r}, k) c_k e^{iE_k t} + \sum_{\tilde{k}} V_{\mu}^{(D)}(\mathbf{r}, \tilde{k}) b_{\tilde{k}} e^{-iE_{\tilde{k}} t}
\]

, whereby

\[
\mathbf{H}_{\mu,\mu'}^{(D)} U_{\mu}^{(D)}(\mathbf{r}, k) = E_k U_{\mu}^{(D)}(\mathbf{r}, k)
\]

\[
\mathbf{H}_{\mu,\mu'}^{(D)} V_{\mu}^{(D)}(\mathbf{r}, \tilde{k}) = -E_{\tilde{k}} V_{\mu}^{(D)}(\mathbf{r}, \tilde{k})
\]

In (14) the expansion coefficients, referred to as \( c_k \) and \( b_{\tilde{k}} \), are c-numbers, obtainable from a prescribed amplitude \( \Psi_{\mu}^{(D)}(\mathbf{r}) \) at an initial time \( t = 0 \) making use of the orthonormality
of those eigenfunctions. Mind the labels $k$ and $\tilde{k}$, counting the positive-energy eigenmodes $U_{\mu}^{(D)}(r,k)$ or rather the negative-energy eigenmodes $V_{\mu}^{(D)}(r,\tilde{k})$ of the Dirac Hamiltonian, have in the presence of an electrostatic field $\mathbf{E}(r) = -\nabla \Phi(r)$ possibly different codomains (for instance if there exist bound states). Because a complete set of orthonormal eigenfunctions of the Dirac Hamiltonian comprises naturally the positive- and the negative-energy eigenstates jointly, the position operator in the Dirac theory, if defined by the operation of multiplication

$$x_a \Psi_{\mu}^{(D)}(r,t) = r_a \Psi_{\mu}^{(D)}(r,t)$$

(16)

is not an operator defined over well defined states of a particle, since in the evaluation of the expectation value $\langle \Psi^{(D)} | x_a | \Psi^{(D)} \rangle$ of the position operator in a given Dirac state $| \Psi^{(D)} \rangle$ the positive-energy solutions interfere with the (seemingly unphysical) negative-energy solutions. The origin of this difficulty is the assumed consent of the Dirac amplitude $\Psi_{\mu}^{(D)}(r,t)$ being a probability amplitude for particles just like in nonrelativistic Schrödinger quantum mechanics, which is plainly wrong, as has been first revealed by the analysis of the meaning of locality in quantum mechanics by Newton and Wigner [1]. For a brilliantly witty discussion of this point, already elucidated in pioneering work by Foldy and Wouthuysen [2], we refer to Costella and McKellar [3]. Indeed interpreting $\Psi_{\mu}^{(D)}(r,t)$ as a probability amplitude gives cause to several well known absurdities, for instance the components of the “velocity” operator in the Heisenberg picture do not commute and have eigenvalues equal to $\pm c$, see [16], [17], [20]. Related to this is the concession that the phenomenon of the highly oscillatory “Zitterbewegung”, sometimes discussed as an inevitable property of the relativistic electron, is actually not a physical property of a moving particle with attributes mass, charge and spin [3].

III. THE NEWTON-WIGNER AMPLITUDE AND THE NOTION OF ENERGY SEPARATION

A physically correct probability amplitude, that in the style of the discussion given by Costella and McKellar [3] we refer to in what follows as the Newton-Wigner amplitude $\Psi_{\mu}^{(NW)}(r,t)$, can be constructed from the four-component Dirac amplitude $\Psi_{\mu}^{(D)}(r,t)$ by a
suitable unitary transformation $T$, such that
\[ \Psi^{(NW)}_\mu(r, t) = T_{\mu, \mu'} \Psi^{(D)}_{\mu'}(r, t) \] (17)
permits a meaningful expectation value in particular for the operators of position, velocity, spin and also orbital angular momentum \[2, 3\].

To this end one looks first for a unitary transformation $T$ requiring the transformed Dirac Hamiltonian
\[ H^{(NW)} \equiv TH^{(D)}T^\dagger \] (18)
be an even operator, so that
\[ \tilde{H}^{(NW)} \beta = \beta \tilde{H}^{(NW)} \] (19)
Taken by itself the criterion (19) only ensures, minding our choice $\beta = \text{diag}\{1, 1, -1, -1\}$ in Dirac-Pauli representation, that $H^{(NW)}$ assumes a block-diagonal guise, but that doesn’t warrant $H^{(NW)}$ being energy-separating, the latter notion first introduced by Eriksen and Kolsrud \[14\]. Possibly the criterion is better understood introducing abstract bra- and ket-notation, so that $U^{(D)}(r, k) = \langle r, \mu | U^{(D)}_k \rangle$ and $V^{(D)}(r, \tilde{k}) = \langle r, \mu | V^{(D)}_{\tilde{k}} \rangle$. Introducing the spectral representations of the Dirac Hamiltonian and it’s associated energy-sign operator $\Lambda^{(D)}$ in the basis of Dirac eigenstates,
\[ H^{(D)} = \sum_k E_k \left| U^{(D)}_k \right\rangle \left\langle U^{(D)}_k \right| + \sum_k \left( -E_\tilde{k} \right) \left| V^{(D)}_{\tilde{k}} \right\rangle \left\langle V^{(D)}_{\tilde{k}} \right| \] (20)
\[ \Lambda^{(D)} = \sum_k \left| U^{(D)}_k \right\rangle \left\langle U^{(D)}_k \right| - \sum_k \left| V^{(D)}_{\tilde{k}} \right\rangle \left\langle V^{(D)}_{\tilde{k}} \right| = \frac{H^{(D)}}{\sqrt{H^{(D)}H^{(D)}}} \] (21)
, it follows at once in terms of the unitary transformed Dirac eigenstates
\[ \left| U^{(NW)}_k \right\rangle = T \left| U^{(D)}_k \right\rangle \] (22)
\[ \left| V^{(NW)}_{\tilde{k}} \right\rangle = T \left| V^{(D)}_{\tilde{k}} \right\rangle \]
for the Dirac $\beta$-operator the representation
\[ \beta = T \Lambda^{(D)} T^\dagger = \frac{H^{(NW)}}{\sqrt{H^{(NW)}H^{(NW)}}} \] (23)
In reverse order, the Newton-Wigner Hamiltonian $H^{(NW)}$ is defined as being one of a kind among all unitary transformed Hamiltonians with block-diagonal guise, satisfying additionally the identity \[14\]
\[ H^{(NW)} = \beta \sqrt{H^{(NW)}H^{(NW)}} \] (24)
As a direct consequence of (24) being true then
\[
(0_{4 \times 1})_{\mu} = \left( H^{\text{NW}}_{\mu} - \beta \sqrt{H^{\text{NW}}_{\mu}} H^{\text{NW}}_{\mu} \right) U^{\text{NW}}_{\mu,\mu'} (r, k) = E_k \left( \hat{1}_{4 \times 4} - \beta \right)_{\mu,\mu'} U^{\text{NW}}_{\mu,\mu'} (r, k)
\] (25)
\[
(0_{4 \times 1})_{\mu} = \left( H^{\text{NW}}_{\mu} - \beta \sqrt{H^{\text{NW}}_{\mu}} H^{\text{NW}}_{\mu} \right) V^{\text{NW}}_{\mu,\mu'} (r, \tilde{k}) = (-E_{\tilde{k}}) \left( \hat{1}_{4 \times 4} + \beta \right)_{\mu,\mu'} V^{\text{NW}}_{\mu,\mu'} (r, \tilde{k})
\] (26)

Assuming nonvanishing eigenvalues, \( E_k \neq 0 \) and \( E_{\tilde{k}} \neq 0 \), this entails at once, minding \( \beta \) being diagonal in Dirac-Pauli representation, that \( U^{\text{NW}}_{\mu} (r, k) \equiv 0 \) regarding the lower components \( \mu = 3, 4 \) and \( V^{\text{NW}}_{\mu} (r, \tilde{k}) \equiv 0 \) regarding the upper components \( \mu = 1, 2 \). This distinguishing feature indeed is the essence of the said energy-separating property of the Newton-Wigner representation, it being the representation in which the operators position, velocity, orbital angular momentum and spin of the free theory are agreeable to physical intuition just like in classical physics [2, 3, 21].

Perhaps, the physical meaning of the concept of energy-separation becomes more comprehensible if one applies the unitary transformation \( T \) to the Dirac-amplitude (14) and rewrites the Newton-Wigner amplitude (17) now with the transformed Dirac-eigenstates (22) as
\[
\Psi^{\text{NW}}_{\mu} (r, t) = \sum_k U^{\text{NW}}_{\mu} (r, k) c_k e^{iE_k t} + \sum_{\tilde{k}} V^{\text{NW}}_{\mu} (r, \tilde{k}) b_{\tilde{k}} e^{-iE_{\tilde{k}} t} \] (27)
Expressely stated, \( \Psi^{\text{NW}}_{\mu} (r, t) \) assumes in consequence of \( U^{\text{NW}}_{\mu} (r, k) \equiv 0 \) for \( \mu = 3, 4 \) and \( V^{\text{NW}}_{\mu} (r, k) \equiv 0 \) for \( \mu = 1, 2 \) the guise
\[
\Psi^{\text{NW}}_{\mu} (r, t) = \begin{pmatrix}
\psi_+ (r, t) \\
\psi_- (r, t) \\
0 \\
0
\end{pmatrix}
\]
\[
+ \begin{pmatrix}
0 \\
0 \\
\chi_+ (r, t) \\
\chi_- (r, t)
\end{pmatrix}
\] (28)

Writing \( H^{\text{NW}} \) as well in explicit \( 2 \times 2 \) block notation,
\[
H^{\text{NW}} \equiv \begin{pmatrix}
H_{2 \times 2}^{(e)} & 0_{2 \times 2} \\
0_{2 \times 2} & -H_{2 \times 2}^{(p)}
\end{pmatrix}
\] (29)
, the resulting equations of motion governing the time evolution of the two-component amplitudes \( \psi_{\sigma} (r, t) \) and \( \chi_{\sigma} (r, t) \) are now by construction forever propagating without any
interference of positive- and negative-energy states, i.e.

\[ i\hbar \partial_t \psi_\sigma (r, t) = \left( H_{2\times2}^{(e)} \right)_{\sigma,\sigma'} \psi_{\sigma'} (r, t) \]  
\[ i\hbar \partial_t \chi_\sigma (r, t) = - \left( H_{2\times2}^{(p)} \right)_{\sigma,\sigma'} \chi_{\sigma'} (r, t) \]

\[ \sigma, \sigma' \in \{ +, - \} \]  

These are Schrödinger-Pauli type equations, whereas the amplitude \( \psi_\sigma (r, t) \) describing the electron as a particle (wave packet) with attributes mass \( m \), spin \( \pm \frac{\hbar}{2} \) and charge \( q_e = -|e| \) is composed exclusively of positive-energy eigenfunctions \( U_{\mu}^{(NW)} (r, k) \). Correlating with this, as the amplitude \( \chi_\sigma (r, t) \) is composed solely of negative-energy eigenfunctions \( V_{\mu}^{(NW)} (r, \tilde{k}) \), it has been given a physical interpretation already by Dirac himself via charge conjugation, so that \( \chi^\ast_{-\sigma} (r, t) \) is describing the positron as an “anti-particle” (wave packet) with attributes mass \( m \), spin \( \mp \frac{\hbar}{2} \) and opposite charge \( q_p = |e| \), albeit Dirac’s hole picture implicitly already involved a quantum field theory context. By this means the specific unitary transformation \( T \), that leads from the Dirac Hamiltonian \( H^{(D)} \) to the energy-separating Hamiltonian \( H^{(NW)} \), enables to bare the roots of Dirac’s discovery of antimatter.

To illustrate the concept of energy separation from a different point of view, assume a certain unitary transformation \( U \) brought the Dirac Hamiltonian \( H^{(D)} \) to a block-diagonal guise

\[ H^{(U)} = U H^{(D)} U^\dagger = \begin{pmatrix} H_{2\times2}^{(I)} & 0_{2\times2} \\ 0_{2\times2} & H_{2\times2}^{(II)} \end{pmatrix} \]  

(31)

Now by construction \( H^{(U)} \beta = \beta H^{(U)} \), yet it is not ensured the upper block operator \( H_{2\times2}^{(I)} \) being positive definite and concurrently the lower block operator \( H_{2\times2}^{(II)} \) being negative definite. This entails that a four-component amplitude \( \Psi_{\mu,(I)}^{(D)} (r, t) \), say generated by applying the inverse unitary transformation \( U^\dagger \) to a two-component amplitude \( \psi^{(I)}_\sigma (r, t) \) being solely composed of the eigenfunctions of \( H_{2\times2}^{(I)} \), i.e.

\[ \Psi_{\mu,(I)}^{(D)} (r, t) = \left( U^\dagger \right)_{\mu,\sigma} \psi^{(I)}_\sigma (r, t) \]  

(32)

, certainly represents a solution of the Dirac equation (11). Yet it (conceivably) comprises a linear combination of positive energy and negative energy eigenfunctions of \( H^{(D)} \) just like in (14). Such a unitary transformation \( U \) is, of course, not energy-separating.

But even if \( H_{2\times2}^{(I)} \) in (31) was positive definite and \( H_{2\times2}^{(II)} \) in (31) was negative definite, there
exists an ambiguity, as any *additional* unitary transformation \( \mathbf{N} \), taking a shape

\[
\mathbf{N} = \begin{pmatrix}
\mathbf{N}^{(I)}_{2 \times 2}, & 0_{2 \times 2} \\
0_{2 \times 2}, & \mathbf{N}^{(II)}_{2 \times 2}
\end{pmatrix}
\]  

(33)

, now changes the \( 2 \times 2 \)-subblocks \( \mathbf{H}^{(I)}_{2 \times 2} \) and \( \mathbf{H}^{(II)}_{2 \times 2} \) in (31) into equivalent unitary transformed operators \( \mathbf{N}^{(I)}_{2 \times 2} \mathbf{H}^{(I)}_{2 \times 2} \left( \mathbf{N}^{(I)}_{2 \times 2} \right)^\dagger \) and \( \mathbf{N}^{(II)}_{2 \times 2} \mathbf{H}^{(II)}_{2 \times 2} \left( \mathbf{N}^{(II)}_{2 \times 2} \right)^\dagger \). So then the question arises, how to remove that ambiguity inherent to any such unitary transformation \( \mathbf{V} = \mathbf{N} \mathbf{U} \)? In what follows we present a flow equation approach enabling to construct for the Dirac Hamiltonian it’s unambiguous energy-separating unitary equivalent, the Wigner-Newton Hamiltonian.

Last not least, while the Dirac Hamiltonian \( \mathbf{H}^{(D)} \) is unique due to its linearity and minimal coupling to external fields, the Newton-Wigner Hamiltonian \( \mathbf{H}^{(NW)} \) is the only one enabling a meaningful nonrelativistic limit in terms of particles and anti-particles moving as completely separated entities along their individual trajectories, as any bubble chamber track reveals. Unfortunately, a disadvantage of this very useful property of \( \mathbf{H}^{(NW)} \) is that locality of the Dirac-Hamiltonian \( \mathbf{H}^{(D)} \), as it comprises only first order differential operators, has been traded off for a nonlocal operator, with \( \sqrt{\mathbf{H}^{(NW)} \mathbf{H}^{(NW)}} \) essentially being an integral kernel. Further, in marked contrast to the Dirac equation, the unitary equivalent equations of motion (30) based on the square root operator (29) are obviously not covariant. Damage of covariance regarding conformable square root operators has been discussed before by several authors dealing, for instance, with the easier problem of relativistic spin-0 particles [22] [23] [24]. But in view of obtaining a suitable starting point for approximations endeavouring to the quantum mechanics of nonrelativistic particles that flaw has little concernment.

IV. EXTERNAL MAGNETOSTATIC FIELD

In the special case the Dirac particle is moving solely in the presence of a magnetostatic field,

\[
\mathbf{H}^{(D)}_{0} = m c^2 \beta + c a_b \Pi_b
\]  

(34)

the unitary transformation \( \mathbf{T}_0 \) transforming \( \mathbf{H}^{(D)}_{0} \) to \( \mathbf{H}^{(NW)}_{0} \) is known exactly in terms of a straightforward generalization [4, 5] of the result obtained afore by Foldy and Wouthuysen.
for the case of a free (translational invariant) Dirac Hamiltonian [2]:

\[
T_0 = \sqrt{\frac{1}{2}} \left( 1_{4 \times 4} + \frac{mc^2}{\sqrt{H_0^{(D)} \circ H_0^{(D)}}} \right) + \beta \frac{\alpha \Pi_b}{\sqrt{(\alpha \Pi_b)^2}} \sqrt{\frac{1}{2}} \left( 1_{4 \times 4} - \frac{mc^2}{\sqrt{H_0^{(D)} \circ H_0^{(D)}}} \right)
\]  

(35)

In this case the following explicit guise for the Newton-Wigner Hamiltonian is obtained

\[
H_0^{(NW)} = T_0 H_0^{(D)} T_0^\dagger = \beta \sqrt{H_0^{(D)} \circ H_0^{(D)}}
\]

(36)

\[
= \beta mc^2 \cdot \sqrt{1_{4 \times 4} + \frac{2}{mc^2} (1_{2 \times 2} \otimes H_{2 \times 2}^{(SP)})}
\]

, with \( H_{2 \times 2}^{(SP)} \) the common Schrödinger-Pauli Hamiltonian,

\[
H_{2 \times 2}^{(SP)} = \frac{\Pi_b \Pi_b}{2m} 1_{2 \times 2} - \frac{q \hbar}{2m} D_{b}^{(ext)} \sigma_b^{(P)}
\]

(37)

, now describing (in constant magnetic field) the Landau levels of a nonrelativistic electron. From (36) a meaningful nonrelativistic Hamiltonian together with the lowest relativistic correction on the energy scale of fine structure is readily obtained considering the rest energy \( mc^2 \) of the electron as the predominant term:

\[
\beta H_0^{(NW)} = 1_{2 \times 2} \otimes \left( mc^2 1_{2 \times 2} + H_{2 \times 2}^{(SP)} - \frac{1}{2mc^2} H_{2 \times 2}^{(SP)} H_{2 \times 2}^{(SP)} + \ldots \right)
\]

(38)

In the expansion (14) of the four component Dirac amplitude, the positive-energy eigenmodes \( U_\mu (r, k) \), if regarded separately from the complementing negative-energy eigenmodes \( V_\mu (r, \tilde{k}) \), do not represent a complete set of eigenfunctions, while the NW-eigenmodes \( U_\mu^{(NW)} (r, k) \) and \( V_\mu^{(NW)} (r, \tilde{k}) \) of \( H_0^{(NW)} \) are directly connected to the complete and orthonormal set of the two-component eigenmodes \( u_\sigma^{(SP)} (r, k) \) of \( H_{2 \times 2}^{(SP)} \). Now restricting to the nonrelativistic sector then the associated eigenfunctions \( u_\sigma^{(SP)} (r, k) \) of \( H_{2 \times 2}^{(SP)} \) and for that matter the eigenfunctions \( U_\mu^{(NW)} (r, k) \) and \( V_\mu^{(NW)} (r, \tilde{k}) \) of \( H_0^{(NW)} \) will be slowly varying functions on the scale of the Compton wavelength \( \lambda_C \), thus providing an eminently suitable starting point for obtaining a nonrelativistic approximation to matrix-elements originally build with four-component Dirac amplitudes.

As a final remark, given a complete system of eigenfunction of \( H_{2 \times 2}^{(SP)} \), a corresponding complete system of eigenfunctions of \( H_0^{(D)} \) can be readily generated upon application of the inverse transformation \( T^\dagger \) applied to those eigenfunctions of \( H_{2 \times 2}^{(SP)} \).
V. THE BETA-FLOW EQUATION TRANSFORMING THE DIRAC $\beta$ INTO THE ENERGY-SIGN OPERATOR $\Lambda^{(D)}$ FOR A DIRAC HAMILTONIAN WITH COUPLING TO ELECTROSTATIC AND MAGNETOSTATIC FIELDS

If a charge carrying Dirac fermion moves in the presence of magnetostatic and electrostatic fields superposed, it is generally accepted to be difficult \[5, 14, 25, 26, 27\] obtaining the unitary transformation $T$, and in this way the Newton-Wigner Hamiltonian $H^{(NW)}$ from a Dirac Hamiltonian $H^{(D)}$ as stated in (12). Let us agree on terming operators $O$ as being odd and operators $E$ as being even, iff

$$ O\beta = -\beta O $$
$$ E\beta = \beta E $$

We aim in this section at constructing a flow striving from a general Dirac Hamiltonian

$$ H^{(D)} = \beta mc^2 + O + E $$

(40)

towards the corresponding Newton-Wigner Hamiltonian $H^{(NW)}$. For example, a well known extension of the Dirac Hamiltonian in external fields, as stated afore in (12), takes into account, besides mass $m$ and charge $q_e$, further phenomenological attributes for the spin-$\frac{1}{2}$ “particles” like an intrinsic anomalous magnetic moment $\mu_M$ or even an intrinsic electric dipole moment $d_E$, see for instance \[28\]. In this case

$$ O = c\alpha_b\Pi_b + i\beta\alpha_b \left( \frac{\mu M}{c} E^{(ext)}_b - cd_E B^{(ext)}_b \right) $$

(41)
$$ E = q_e\Phi(x) - \frac{\Pi_b}{mc} \left( \mu_M B^{(ext)}_b + d_E E^{(ext)}_b \right) $$

(42)

Of course, with $d_E \neq 0$ then (spatial) parity is not conserved \[29\]. Whereas in standard QED for sure $d_E \equiv 0 \ [29]$, instead in electroweak theory $d_E \neq 0$ appears quite reasonable. For a thorough discussion see \[30, 21\].

In order to determine the exact solution to the nonlinear flow equation (4) with generator $\eta(s) = [\beta, H(s)]$, the idea is to look for an operator $Z(s)$ representing a continuous unitary transformation of the Dirac matrix $\beta$ by solving the flow equation

$$ \frac{d}{ds} Z(s) = [\omega(s), Z(s)] $$
$$ Z(0) = \beta $$

(43)
, and in particular to choose the generator $\omega(s)$ of that “beta-flow” in such a way, that the limiting value $Z(\infty)$ commutes with the original Dirac Hamiltonian $\tilde{H}(D)$

$$\left[\tilde{H}(D), Z(\infty)\right] = 0_{4\times4} \quad (44)$$

Along the line of reasoning presented afore in (4) a suitable antisymmetric generator of such a beta-flow emerges as

$$\omega(s) = \left[\tilde{H}(D), Z(s)\right] \quad (45)$$

whereby

$$\tilde{H}^{(D)} = \frac{1}{mc^2}H^{(D)} = \beta + \tilde{\mathcal{E}} + \tilde{\mathcal{O}} \quad (46)$$

If (43) could be solved for $Z(s)$, then the generator $\omega(s)$ was known explicitely and the unitary transformation of $\beta$ could be represented as

$$Z(s) = V(s)\beta V(s)^\dagger \quad (47)$$

whereby the unitary transformation $V(s)$ solves

$$\frac{d}{ds}V(s) = \omega(s)V(s) \quad (48)$$

$$V(0) = 1_{4\times4}$$

And because the transformation $V(s)$ is unitary, of course there holds

$$\beta \beta = Z(s)Z(s) = Z(\infty)Z(\infty) = 1_{4\times4} \quad (49)$$

Consideration should be given to an ambiguity regarding the representation of $Z(s)$ in (47) with such a unitary transformation $V(s)$. Indeed, with $N(s)$ another unitary operator with attributes

$$N(s)\beta = \beta N(s) \quad (50)$$

, then instead of (47) one finds for $Z(s)$ as well the entirely equivalent representation

$$Z(s) = U(s)\beta U(s)^\dagger \quad (51)$$

$$V(s) = U(s)N(s)$$

$$U(0)N(0) = 1_{4\times4}$$

So, even if $Z(s)$ was known exactly, compliant with the representation (47) said unitary transformation $V(s)$ in (51) cannot be determined any better up to an undetermined block-diagonal factor $N(s)$. 

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VI. EXACT SOLUTION OF BETA-FLOW EQUATION

With $\omega(s)$ as specified in (45) the flow equation (43) determining $Z(s)$ reads

$$\frac{d}{ds}Z(s) = \left[\tilde{H}^{(D)}, Z(s)\right], Z(s)$$  \hspace{1cm} (52)

$$Z(0) = \beta$$  \hspace{1cm} (53)

Evaluation of the double commutator gives

$$\left[\left[\tilde{H}^{(D)}, Z(s)\right], Z(s)\right] = \tilde{H}^{(D)}Z(s)Z(s) - 2Z(s)\tilde{H}^{(D)}Z(s) + Z(s)Z(s)\tilde{H}^{(D)}$$  \hspace{1cm} (54)

Because of (49) then (54) simplifies and the differential equation (52) reads

$$\frac{1}{2} \frac{d}{ds}Z(s) = \tilde{H}^{(D)} - Z(s)\tilde{H}^{(D)}Z(s)Z(0)$$  \hspace{1cm} (55)

Serendipitously this being a matrix Riccati equation [32], we can find an exact solution to this initial value problem in the guise

$$Z(s) = W(s)\beta W^{-1}(s)$$  \hspace{1cm} (56)

, with

$$W(s) = C(s)\beta + S(s)$$  \hspace{1cm} (57)

$$C(s) = \cosh\left(2s\tilde{H}^{(D)}\right)$$

$$S(s) = \sinh\left(2s\tilde{H}^{(D)}\right)$$

Despite $\beta\tilde{H}^{(D)} \neq \tilde{H}^{(D)}\beta$, there holds as an identity

$$\beta S(s)S(s) + C(s)C(s)\beta = S(s)S(s)\beta + \beta C(s)C(s)$$  \hspace{1cm} (58)

, and therefore

$$W^\dagger(s)W(s)\beta = \beta W^\dagger(s)W(s)$$  \hspace{1cm} (59)

With that said

$$Z(s) = Z^\dagger(s)$$  \hspace{1cm} (60)

, and in this way

$$Z(s)Z^\dagger(s) = Z^\dagger(s)Z(s) = Z(s)Z(s) = 1_{4\times4}$$  \hspace{1cm} (61)
, thus validating in accord with the representation (47) the operator \( Z(s) \) being unitary (and involutive as well). With \( \Lambda(D) \) the energy-sign operator (21) in the basis of Dirac eigenstates, there holds

\[
\lim_{s \to \infty} C^{-1}(s) S(s) = \lim_{s \to \infty} \frac{\beta}{\sqrt{\tilde{M}(D) \tilde{M}(D)}} \tanh \left( 2s \sqrt{\tilde{M}(D) \tilde{M}(D)} \right) = \Lambda(D)
\]

, and thus for \( s \to \infty \) a meaningful limiting value of \( Z(s) \) identical to the energy-sign operator \( \Lambda(D) \) exists:

\[
Z(\infty) = \lim_{s \to \infty} Z(s) = \lim_{s \to \infty} \left( C(s) \left( \beta + C^{-1}(s) S(s) \right) \beta \left( \beta + C^{-1}(s) S(s) \right)^{-1} C^{-1}(s) \right) = \lim_{s \to \infty} \left( C(s) \left( \beta + \Lambda(D) \right) \beta \left( \beta + \Lambda(D) \right)^{-1} C^{-1}(s) \right) = \Lambda(D)
\]

VII. CONSTRUCTION OF UNITARY TRANSFORMATION \( V(s) \)

Even though the operator \( Z(s) \) in (56) is the exact solution of the beta-flow (52), this doesn’t concurrently determine the unitary transformation \( V(s) \) in the representation (47). Of course, \( W^\dagger(s) W(s) \) being positive definite then a unitary operator \( U^{(P)}(s) \) related to the polar decomposition of the operator \( W(s) \) can be identified in the guise [33]

\[
U^{(P)}(s) = W(s) \left( W^\dagger(s) W(s) \right)^{-\frac{1}{2}}
\]

And with help of (59) it follows then

\[
Z(s) = U^{(P)}(s) \beta \left( U^{(P)}(s) \right)^\dagger
\]

, with \( U^{(P)}(s) \) (after re-arrangement of the square root term) given by

\[
U^{(P)}(s) = (C(s) \beta + S(s)) \left( \beta C(s) + S(s) \right) \left( C(s) \beta + S(s) \right)^{-\frac{1}{2}}
\]

But now a complicacy arises, as the identification of (66) with the searched for unitary transformation \( V(s) \), setting

\[
V(s) \equiv U^{(P)}(s) \beta
\]
in view of the posed initial value (48), actually is expedient only iff
\[
[\beta, \sqrt{\tilde{H}^{(D)}\tilde{H}^{(D)}}] = 0_{4\times 4}
\] (68)

This special constraint immediately implying \(C(s)\beta = \beta C(s)\), only then a meaningful limit of \(U^{(P)}(s)\) for \(s \to \infty\) is readily obtained
\[
U^{(P)}(\infty) = \frac{\beta + \Lambda^{(D)}}{\sqrt{\beta + \Lambda^{(D)}}^2}
\] (69)

Unfortunately, the restriction (68) is not fitting in at all, say, with the presence of an external electrostatic potential \(\Phi(r) \neq 0\) in the Dirac Hamiltonian, as the square \(\tilde{H}^{(D)}\tilde{H}^{(D)}\) then also comprises odd terms (anti-commuting with \(\beta\)). Thus, except in (special) cases when (68) applies, as concerns for instance the Dirac Hamiltonian \(\tilde{H}_0^{(D)}\) stated in (34), for a general Dirac Hamiltonian \(\tilde{H}^{(D)}\) the limiting value of \(U^{(P)}(s)\) indeed remains indeterminable due to our ignorance how to find the limiting value of terms like \(C^{-1}(s)\beta S(s)\) for \(s \to \infty\). This symptom reveals the polar decomposition (64) being pointless if (68) ceases to be valid. Briefly speaking, that way we cannot find the searched for unitary transformation for a general Dirac Hamiltonian, even though the limiting value \(Z(s)\) for \(s \to \infty\) has according to (63) already an assigned value.

Progress comes, accepting (for the moment being) a simplified way of writing \(Z \equiv Z(s)\), from the observation
\[
(\beta + Z)\beta = Z(\beta + Z)
\]
\[
[\beta, (\beta Z + Z\beta)] = 0_{4\times 4} = [Z, (\beta Z + Z\beta)]
\]

, so that
\[
Z(s) = Z(\beta + Z)(\beta + Z)^{-1}
\]
\[
= (\beta + Z)\beta(\beta + Z)^{-1}
\]
\[
= (\beta + Z)\beta(\beta + Z)^{-2}(\beta + Z)
\]

The operator \(\beta + Z\) being hermitean (and excluding zero as an eigenvalue of that operator), then for sure \((\beta + Z)^2\) is positive definite, so that
\[
(\beta + Z)^{-2} = \left(\sqrt{(\beta + Z)^2}\sqrt{(\beta + Z)^2}\right)^{-1}
\] (72)
On these grounds there follows now the representation

\[ Z(s) = U(s) \beta U^\dagger(s) \]  

(73), with \( U(s) \) being unitary and built-up in terms of the exact solution \( Z(s) \) as given in (56):

\[ U(s) = \frac{\beta + Z(s)}{\sqrt{(\beta + Z(s))^2}} \]  

(74)

\[ U(0) = \beta \]  

(75)

With the known limiting value (63) then

\[ U(\infty) = \frac{\beta + \Lambda^{(D)}}{\sqrt{(\beta + \Lambda^{(D)})^2}} \]  

(76)

Remarkably enough, even though the operator \( U(P)(s) \) introduced in (64) has only under the special premise (68) for \( s \to \infty \) a definite limit (69), nonetheless that limiting value coincides with the generally valid result (76). Yet, in view of the posed initial value (48), the searched for unitary transformation is \textit{not} \( U(s) \), but

\[ V(s) \equiv U(s) \beta = \frac{\beta + Z(s)}{\sqrt{(\beta + Z(s))^2}} \beta \]  

(77)

So in point of fact with \( V(s) \) given in (77) we have

\[ Z(s) = V(s) \beta V^\dagger(s) \]  

(78)

\[ V(0) = 1_{4 \times 4} \]

\[ V(s) V^\dagger(s) = 1_{4 \times 4} = V^\dagger(s) V(s) \]

Notably, based on the identities

\[ U(s) U(s) = 1_{4 \times 4} \]  

(79)

\[ \beta U(s) = U(s) Z(s) \]

, there holds for this particular transformation (77) as well

\[ V(s) V(s) = U(s) \beta U(s) \beta \]  

(80)

\[ = U(s) U(s) Z(s) \beta \]

\[ = Z(s) \beta \]
VIII. RETRIEVAL OF THE NEWTON-WIGNER HAMILTONIAN

The basic cause of the unitary transformation $V(s)$ stated in (77) being for $s \to \infty$ in fact energy-separating, is the identity

$$V(\infty)\beta V^\dagger(\infty) = Z(\infty) = \Lambda^{(D)}$$  \hspace{1cm} (81)

The sought for unitary transformation $T$ that maps the Dirac Hamiltonian $H^{(D)}$ to the Newton-Wigner Hamiltonian $H^{(NW)}$ we thus identify directly from (77) as

$$T \equiv V^\dagger(\infty) = \beta \frac{\beta + \Lambda^{(D)}}{\sqrt{(\beta + \Lambda^{(D)})^2}}$$  \hspace{1cm} (82)

Obviously there holds now

$$\beta T = T \Lambda^{(D)}$$  \hspace{1cm} (83)

Applying $T$ to positive energy eigenstates $|U_k^{(D)}\rangle$ of $\tilde{H}^{(D)}$, respectively applying $T$ to negative energy eigenstates $|V_k^{(D)}\rangle$ of $\tilde{H}^{(D)}$, it is manifest that the unitary transformation $T$ is as well energy-separating:

$$\beta \left( T |U_k^{(D)}\rangle \right) = T \Lambda^{(D)} |U_k^{(D)}\rangle = +T |U_k^{(D)}\rangle$$

$$\beta \left( T |V_k^{(D)}\rangle \right) = T \Lambda^{(D)} |V_k^{(D)}\rangle = -T |V_k^{(D)}\rangle$$  \hspace{1cm} (84)

Indeed, due to (63) we have

$$\sqrt{H^{(D)}H^{(D)}} = \Lambda^{(D)}H^{(D)}$$

$$= Z(\infty)H^{(D)}$$

$$= (V(\infty)\beta V^\dagger(\infty))H^{(D)}$$

$$= (T^\dagger\beta T)H^{(D)}$$

, and so it follows

$$\sqrt{(TH^{(D)}T^\dagger)(TH^{(D)}T^\dagger)} = T \left( \sqrt{H^{(D)}H^{(D)}} \right) T^\dagger$$

$$= T(T^\dagger\beta T)H^{(D)}T^\dagger$$

$$= \beta (TH^{(D)}T^\dagger)$$  \hspace{1cm} (86)

Writing $\Lambda^{(D)}H^{(D)} = \sqrt{H^{(D)}H^{(D)}} = H^{(D)}\Lambda^{(D)}$, then directly from (85) along the lines indicated in (86)

$$\beta (TH^{(D)}T^\dagger) = (TH^{(D)}T^\dagger)\beta$$  \hspace{1cm} (87)
Comparing (24) with (86) we thus identify, among all unitary transformations producing merely a $2 \times 2$ - block-diagonalization of the Dirac-Pauli Hamiltonian, the even and energy-separating Newton-Wigner Hamiltonian being

$$H^{(NW)} = T H^{(D)} T^\dagger$$

whereas $T$ is the specific unitary transformation stated in (82).

IX. ERIKSEN TRANSFORMATION

In pioneering work Eriksen [5] fixed the unitary transformation $U_E$ bearing his name, by postulating

$$U_E^\dagger \beta = \beta U_E$$

From this he concluded

$$A^{(D)} = U_E^\dagger \beta U_E = \beta U_E^2$$

, and (excluding $-1$ as an eigenvalue of $\beta A^{(D)}$) obtained [5][34]

$$U_E = \sqrt{\beta A^{(D)}} \equiv \frac{1}{2} \left( 1_{4 \times 4} + \beta A^{(D)} \right)$$

Comparing $U_E$ with our result (82) we readily confirm the limiting value $T = \lim_{s \to \infty} V^\dagger (s)$ being identical to Eriksen’s transformation:

$$T = \beta \frac{\beta + A^{(D)}}{\sqrt{(\beta + A^{(D)})^2}} = U_E$$

X. A LINK BETWEEN THE HAMILTONIAN FLOW AND THE BETA-FLOW

As a general proposition, the solution $H (s)$ to the (nonlinear) Hamiltonian flow equation (4) with generator $\eta (s) = [\beta, H (s)]$ enables a representation in the guise

$$H (s) = V^\dagger (s) \tilde{H}^{(D)} V (s)$$

, whereby $V (s)$ is the afore introduced specific unitary transformation solving the initial value problem (48) with the generator of the beta-flow (43)

$$\omega (s) = \left[ \tilde{H}^{(D)}, Z (s) \right]$$
The validation of (93) follows readily calculating the derivative and minding subsequently (48), (94) and (47). Then

\[ \frac{d}{ds} H(s) = V_\dagger(s) \left[ \tilde{H}^{(D)}, \omega(s) \right] V(s) \]

(95)

\[ = V_\dagger(s) \left( \left[ \tilde{H}^{(D)}, \left[ \tilde{H}^{(D)}, Z(s) \right] \right] \right) V(s) \]

\[ = V_\dagger(s) \left( \begin{pmatrix} \tilde{H}^{(D)} & \tilde{H}^{(D)} (V(s) \beta V_\dagger(s)) \\ -2\tilde{H}^{(D)} (V(s) \beta V_\dagger(s)) & \tilde{H}^{(D)} \end{pmatrix} \right) V(s) \]

\[ = H(s) H(s) \beta - 2H(s) \beta H(s) + \beta H(s) H(s) \]

\[ = \left[ \beta, H(s) \right], H(s) \]

, or else

\[ \frac{d}{ds} H(s) = [\eta(s), H(s)] \]

(96)

\[ \eta(s) = [\beta, H(s)] \]

\[ H(0) = \tilde{H}^{(D)} \]

The ODE obtained for \( H(s) \) this way, with (scaled) initial data \( H(0) = \tilde{H}^{(D)} \), coincides with the Hamiltonian flow (44), thus substantiating the assertion (93). Not unsuspected then, said generators, \( \eta(s) \) for the Hamiltonian flow (96) and \( \omega(s) \) for the associated beta-flow (43), are mutually connected by the same unitary transformation \( V(s) \), i.e. once \( \omega(s) \) is known, then \( \eta(s) \) is known and vice versa

\[ \eta(s) = -V_\dagger(s) \omega(s) V(s) \]

(97)

Indeed

\[ \omega(s) = [H^{(D)}, Z(s)] \]

\[ = [H^{(D)}, V(s) \beta V_\dagger(s)] \]

\[ = H^{(D)} V(s) \beta V_\dagger(s) - V(s) \beta V_\dagger(s) H^{(D)} \]

\[ = V(s) \left( V_\dagger(s) H^{(D)} V(s) \beta - \beta V_\dagger(s) H^{(D)} V(s) \right) V_\dagger(s) \]

\[ = V(s) \left( H(s) \beta - \beta H(s) \right) V_\dagger(s) \]

\[ = -V(s) \left[ \beta, H(s) \right] V_\dagger(s) \]

\[ = -V(s) \eta(s) V_\dagger(s) \]
Notably, upon insertion of the afore obtained exact solution \( Z(s) \) stated in (56) then the generator \( \omega(s) \) being a known function of the flow parameter \( s \), this fact enables to write an explicit (formal though) solution of the linear ODE (48) determining the unitary transformation \( V(s) \) as an \( s \)-ordered exponential

\[
V(s) = T_s \exp \left[ \int_0^s ds' \omega(s') \right]
\]

or else known as the Dyson series \[19\]. Conversely, using unitarity, (48) and reexpressing the generator of the beta-flow \( \omega(s) \) in terms of \( \eta(s) \) using the identity (97), it follows at once

\[
0 = V^\dagger(s) \frac{d}{ds} \left( V(s) V^\dagger(s) \right)
= V^\dagger(s) \left( \frac{d}{ds} V(s) \right) V^\dagger(s) + \frac{d}{ds} V^\dagger(s)
= \left( V^\dagger(s) \omega(s) V(s) \right) V^\dagger(s) + \frac{d}{ds} V^\dagger(s)
= -\eta(s) V^\dagger(s) + \frac{d}{ds} V^\dagger(s)
\]

, i.e. \( V^\dagger(s) \) solves the ODE

\[
\frac{d}{ds} V^\dagger(s) = \eta(s) V^\dagger(s)
\]

\( \eta(s) \left. \right| V^\dagger(0) = 1_{4\times4} \)

This fact implicates an equivalent representation for the adjoint (or else inverse) operator \( V^\dagger(s) \) in the guise of the Dyson series constructed with the generator \( \eta(s) \) of the Hamiltonian flow (96),

\[
V^\dagger(s) = T_s \exp \left[ \int_0^s ds' \eta(s') \right]
\]

Alas, because \( \left[ \beta, \sqrt{\tilde{H}^{(D)} \tilde{H}^{(D)}} \right] \neq 0 \) for a general Dirac Hamiltonian \( \tilde{H}^{(D)} \) then as well \( \left[ \omega(s_1), \omega(s_2) \right] \neq 0 \), alternatively \( \left[ \eta(s_1), \eta(s_2) \right] \neq 0 \), which feature as a rule prevents an elementary calculation of \( V(s) \) in closed form.

Be that as it may, with a generator \( \omega(s) \) of known identity (94) the explicit solution \( V(s) \) of the linear ODE (48) in the guise of the Dyson series (98) or else the Dyson series (100) buildt with \( \eta(s) \), indeed provides an exact solution to the nonlinear Hamiltonian flow equation (96). Mind however, that due to the afore mentioned ambiguity (51), even though \( H(s) \) as a solution to a double-bracket flow (96) by construction strives for \( s \to \infty \).
IX. THE NEWTON-WIGNER HAMILTONIAN FOR A SPECIAL CLASS OF DIRAC HAMILTONIANS

The afore derived exact result (88) for the Newton-Wigner Hamiltonian is amenable to a substantial simplification for the particular class of (scaled) Dirac-Hamiltonians \( \tilde{H}_0^{(D)} \) exhibiting the exceptional feature

\[
\left[ \beta, \left( \tilde{H}_0^{(D)} \tilde{H}_0^{(D)} \right) \right] = 0_{4 \times 4}
\]

as applies for instance to the Dirac-Hamiltonian (34) for a relativistic particle moving solely in the presence of a static external magnetic field and more generally to every (scaled) Dirac Hamiltonians \( \tilde{H}_0^{(D)} = \beta + \tilde{\xi}_0 + \tilde{O}_0 \) with the property \( \left\{ \tilde{O}_0, \tilde{\xi}_0 \right\} \equiv 0 \). Replacing now everywhere in the exact expression (56) the operator \( \tilde{H}_0^{(D)} \) by \( \tilde{H}_0^{(D)} \), one readily obtains proceeding directly from (56) the result

\[
Z_0 (s) = t_0 (s) \Lambda_0^{(D)}
\]

\[
t_0 (s) = \tanh \left( 2s \sqrt{\tilde{H}_0^{(D)} \tilde{H}_0^{(D)} + \text{artanh} \left( \beta \Lambda_0^{(D)} \right)} \right)
\]

The associated generator \( \omega_0 (s) \) of the beta-flow assumes then the guise

\[
\omega_0 (s) = \left[ \tilde{H}_0^{(D)}, Z_0 (s) \right] = \sqrt{\tilde{H}_0^{(D)} \tilde{H}_0^{(D)}} \left( t_0^\dagger (s) - t_0 (s) \right)
\]

Besides being manifestly odd

\[
\beta \omega_0 (s) = -\omega_0 (s) = \omega_0^\dagger (s).
\]

that generator \( \omega_0 (s) \) has a vanishing commutator at different flow parameter values \( s_1, s_2 \), so that

\[
\left[ \omega_0 (s_1), \omega_0 (s_2) \right] = 0_{4 \times 4}
\]

For details of the reasoning leading to (102) and (103) we refer to [12].
Because with \( \text{(102)} \) the functional dependence of \( \omega_0(s) \) on the flow parameter \( s \) is known, now upon insertion of \( \text{(102)} \) into \( \text{(103)} \) an exact analytical expression for the unitary transformation \( V_0(s) \) can be given, so that

\[
H_0(s) = V_0^\dagger(s) \tilde{H}_0^{(D)} V_0(s)
\]  \( \text{(106)} \)

This is because the ODE defining \( V_0(s) \),

\[
\frac{d}{ds} V_0(s) = \omega_0(s) V_0(s)
\]  \( \text{(107)} \)

\[
V_0(0) = 1_{4\times4}
\]

with \( \omega_0(s) \) as stated in \( \text{(103)} \), can be solved due to \( \text{(105)} \) exactly

\[
V_0(s) = T_s \exp \left[ \int_{s_0}^{s} ds' \omega_0(s') \right] = \exp \left[ \int_{s_0}^{s} ds' \omega_0(s') \right]
\]  \( \text{(108)} \)

Evaluation of the integral indeed gives \( \text{(12)} \)

\[
V_0(s) = \sqrt{Z_0(s)} \beta = \frac{\beta + Z_0(s)}{\sqrt{\beta + Z_0(s)^2}} \beta
\]  \( \text{(109)} \)

, which outcome is in full accordance with the afore derived general result \( \text{(92)} \), obtained by replacing in \( \text{(92)} \) the operator \( \tilde{H}^{(D)} \) by \( \tilde{H}_0^{(D)} \). The limiting value of \( Z_0(s) \) for \( s \to \infty \) as determined from \( \text{(102)} \) being now

\[
Z_0(\infty) = \Lambda_0^{(D)} = \frac{\tilde{H}_0^{(D)}}{\sqrt{\tilde{H}_0^{(D)} \tilde{H}_0^{(D)}}}
\]  \( \text{(110)} \)

Defining \( T_0 \equiv V_0^\dagger(\infty) \), there follows using

\[
\beta T_0 = T_0 \Lambda_0^{(D)}
\]

\[
\Lambda_0^{(D)} \tilde{H}_0^{(D)} = \sqrt{\tilde{H}_0^{(D)} \tilde{H}_0^{(D)}}
\]

that \( \text{(101)} \) implies as well

\[
\left[ T_0, \sqrt{\tilde{H}_0^{(D)} \tilde{H}_0^{(D)}} \right] = 0_{4\times4}
\]  \( \text{(111)} \)

It is then straightforward to show

\[
\tilde{H}_0^{(NW)} = T_0 \tilde{H}_0^{(D)} T_0^\dagger
\]

\[
= \beta (\beta T_0) \tilde{H}_0^{(D)} T_0^\dagger
\]

\[
= \beta \left( T_0 \Lambda_0^{(D)} \right) \tilde{H}_0^{(D)} T_0^\dagger
\]

\[
= \beta T_0 \left( \Lambda_0^{(D)} \tilde{H}_0^{(D)} \right) T_0^\dagger
\]

\[
= \beta T_0 \sqrt{\tilde{H}_0^{(D)} \tilde{H}_0^{(D)}} T_0^\dagger
\]
That way, with \( T_0 T_0^\dagger = 1_{4 \times 4} \) the Newton-Wigner Hamiltonian \( \tilde{H}_0^{(NW)} \) associated with a Dirac Hamiltonian \( \tilde{H}_0^{(D)} \) obeying to (101) assumes the simplified guise

\[
\tilde{H}_0^{(NW)} = \beta \sqrt{\tilde{H}_0^{(D)} \tilde{H}_0^{(D)}}
\]  

(112)

This result coincides with findings obtained first without coupling to external fields by Foldy and Wouthuysen [2]. It applies as well in the presence of a magnetic induction field but excluding any coupling to electric potentials, a result first obtained by Case [4] and using different methods by Eriksen [5]. A more general context where the feature (112) applies is considered in [30, 35, 36, 37, 21].

XII. MANIFESTLY EVEN REPRESENTATION OF THE NEWTON-WIGNER HAMILTONIAN AS A SERIES OF ITERATED COMMUTATORS

The ensuing considerations apply to a Dirac Hamiltonian incorporating static external potentials and/or fields (40). According to what has been said afore, the beta-flow equation (52) transforms the operator \( \beta \) into

\[
Z(s) = V(s) \beta V^\dagger(s)
\]

(113), whereas due to (93) that same unitary operator \( V(s) \) concurrently serves as well to represent the solution to the Hamiltonian flow equation (96)

\[
H(s) = V^\dagger(s) \tilde{H}^{(D)} V(s)
\]

(114)

Writing with anti-symmetric operators \( \Omega_u(s) \) and \( \Omega_g(s) \) now

\[
V(s) = e^{\Omega_u(s)} e^{\Omega_g(s)}
\]

(115)

, whereby \( \Omega_u(s) \) is odd and \( \Omega_g(s) \) is even, then

\[
\Omega_u^\dagger(s) = -\Omega_u(s)
\]

(116)

\[
\beta \Omega_u(s) \beta = -\Omega_u(s)
\]

\[
\Omega_g^\dagger(s) = -\Omega_g(s)
\]

(117)

\[
\beta \Omega_g(s) \beta = +\Omega_g(s)
\]
It follows from (114)

\[ H(s) = e^{-\Omega_g(s)} e^{-\Omega_u(s)} \tilde{H}(D) e^{\Omega_u(s)} e^{\Omega_g(s)} \]  

(118)

, whereas from (113) we obtain

\[ Z(s) = e^{\Omega_u(s)} e^{\Omega_g(s)} \beta e^{-\Omega_g(s)} e^{-\Omega_u(s)} = e^{2\Omega_u(s)} \beta \]  

(119)

, which representation for \( Z(s) \) is inherently consistent with (80). That a factorization like (115) exists follows from a general result in Lie-group theory, understanding the role of the operator \( \beta \) in relations like (117) and (116) essentially being equivalent to the action of an “involutive automorphism” [38,39].

Because the limiting value \( H(\infty) \) of the Hamiltonian flow (4) obeys by construction to \( [\beta, H(\infty)] = 0 \), now the searched for Newton-Wigner (NW) Hamiltonian arises in the guise

\[ \tilde{H}^{(NW)} \equiv e^{+\Omega_g(\infty)} H(\infty) e^{-\Omega_g(\infty)} \]  

(120)

\[ = e^{-\Omega_u(\infty)} \tilde{H}(D) e^{\Omega_u(\infty)} \]  

(121)

If \( H(\infty) \) was obtained, for instance solving the Hamiltonian flow (96) perturbatively along the lines indicated in [11], then for sure \( H(\infty) \) is an even operator, but it is not guaranteed \( H(\infty) \) being energy-separating as well. Seen from another perspective, the unitary transformation performed with the even operator \( e^{+\Omega_g(\infty)} \) in (120) can be regarded, once \( \Omega_g(\infty) \) is known, as a “correction-scheme” that converts the merely block-diagonal (even) limiting value \( H(\infty) \) of the Hamiltonian flow (96) into the unique energy-separating Newton-Wigner Hamiltonian.

Alternatively, \( \tilde{H}^{(NW)} \) may be obtained directly from the unitary transformation (121) performed solely with the odd operator \( \Omega_u(\infty) \). Once \( \Omega_u(\infty) \) is known, then the common BCH-expansion [40] leads to a representation as a series of commutators

\[ \tilde{H}^{(NW)} = \tilde{H}(D) - \left[ \Omega_u(\infty), \tilde{H}(D) \right] + \frac{1}{2!} \left[ \Omega_u(\infty), \left[ \Omega_u(\infty), \tilde{H}(D) \right] \right] + ... \]  

(122)

Here it is important to realize, that a straightforward evaluation of this series of iterated commutators is needlessly complicated, because due to the first line in (121) the operator \( \tilde{H}^{(NW)} \) is unconditionally guaranteed to be even. A considerable simplification thus results
rewriting (121) in the equivalent guise

\[
\tilde{H}^{(NW)} = \frac{1}{2} \left( e^{-\Omega_{u}(\infty)} \tilde{H}^{(D)} e^{\Omega_{u}(\infty)} + \beta e^{-\Omega_{u}(\infty)} \tilde{H}^{(D)} e^{\Omega_{u}(\infty)} \beta \right)
\]

\[
= \frac{1}{2} e^{-\Omega_{u}(\infty)} \tilde{H}^{(D)} e^{\Omega_{u}(\infty)} + \frac{1}{2} e^{\Omega_{u}(\infty)} \left( \beta \tilde{H}^{(D)} \beta \right) e^{-\Omega_{u}(\infty)}
\]

\[
= \frac{1}{2} e^{-\Omega_{u}(\infty)} \left( \beta + \tilde{O} + \mathcal{E} \right) e^{\Omega_{u}(\infty)} + \frac{1}{2} e^{\Omega_{u}(\infty)} \left( \beta - \tilde{O} + \mathcal{E} \right) e^{-\Omega_{u}(\infty)}
\]

\[
= \frac{1}{2} \left( \exp \left( -\text{ad}_{\Omega_{u}(\infty)} \right) + \exp \left( +\text{ad}_{\Omega_{u}(\infty)} \right) \right) \circ \left( \beta + \mathcal{E} \right) - \frac{1}{2} \left( \exp \left( \text{ad}_{\Omega_{u}(\infty)} \right) - \exp \left( -\text{ad}_{\Omega_{u}(\infty)} \right) \right) \circ \tilde{O}
\]

, whereby the symbol \( \text{ad}_X \) denotes here a most useful notation to describe iterated commutators as powers, see for instance [41]. With given operators \( X \) and \( F \) then

\[
\text{ad}_X \circ F = [X,F]
\]

\[
(\text{ad}_X)^2 \circ F = \text{ad}_X \circ [X,F] = [X,[X,F]]
\]

\[
\ldots
\]

\[
(\text{ad}_X)^n \circ F = [X,\ldots[X,[X,F]]]_{n\text{-fold}}
\]

It follows introducing formal power series

\[
\exp (\text{ad}_X) \circ F = \sum_{j=0}^{\infty} \frac{1}{j!} (\text{ad}_X)^j \circ F \equiv e^X F e^{-X}
\]

\[
\cosh (\text{ad}_X) \circ F = \sum_{j=0}^{\infty} \frac{1}{(2j)!} (\text{ad}_X)^{2j} \circ F
\]

\[
\sinh (\text{ad}_X) \circ F = \sum_{j=0}^{\infty} \frac{1}{(2j+1)!} (\text{ad}_X)^{2j+1} \circ F
\]

That way an explicit representation for the (scaled) energy-separating Newton-Wigner Hamiltonian is obtained directly from (123) in the guise of a series of iterated commutators composed solely with the odd operator \( \Omega_{u}(\infty) \), each term in this series expansion being manifestly even

\[
\tilde{H}^{(NW)} = \cosh (\text{ad}_{\Omega_{u}(\infty)}) \circ \left( \beta + \mathcal{E} \right) - \sinh (\text{ad}_{\Omega_{u}(\infty)}) \circ \tilde{O}
\]

(126)
Provided a perturbative expansion for the operator $\Omega_u(\infty)$ could be found, then the associated perturbative expansion for the Newton-Wigner-Hamiltonian as represented by (126) is reduced to evaluating just a few commutators.

XIII. A PERTURBATIVE EXPANSION IN THE STYLE OF MAGNUS FOR THE OPERATORS $\Omega_u(s)$ AND $\Omega_g(s)$ DEFINING $V(s) = e^{\Omega_u(s)} e^{\Omega_g(s)}$

Restriction of the Dirac Hamiltonian $\tilde{H}^{(D)}$ in (12) to the low energy sector of its spectrum suggests a weighting of the respective contributions of the kinetic energy and potential energy terms with regard to a small parameter $\kappa = \frac{v}{c}$ (in what follows $\kappa$ serving as a formal bookkeeping device, so that $\kappa = 1$ at the end of the calculations). Different from [11] though the electric potential term $\mathcal{E}$ is here considered in order of magnitude being comparable to the kinetic energy term $\mathcal{O}_K$ for reasons of consistency with the nonrelativistic limit. This implies (scaled units)

$$\tilde{H}^{(D)} = \beta + \kappa \hat{O} + \kappa^2 \hat{E}$$

(127)

To obtain now a perturbation series expansion of the Newton-Wigner Hamiltonian (126) in powers of $\kappa$ we first aim at obtaining a perturbation expansion of the anti-hermitean operators $\Omega_u(s)$ and $\Omega_g(s)$, those operators in fact being closely connected to the generator $\omega(s)$ of the beta-flow (13) or else to the generator $\eta(s)$ of the Hamiltonian flow (36). To this end let us rewrite the identity (127) in the guise

$$e^{-\Omega_u(s)} \omega(s) e^{\Omega_u(s)} = -e^{\Omega_g(s)} \eta(s) e^{-\Omega_g(s)}$$

(128)

As the generator $\eta(s)$ of the Hamiltonian flow is by construction an odd operator,

$$\eta(s) = [\beta, H(s)]$$

$$\beta \eta(s) + \eta(s) \beta = 0_{4\times4}$$

(129)

and the commutator of an even operator with an odd operator is always odd as well, then the even part of the left hand side in (128) should vanish identically,

$$e^{-\Omega_u(s)} \omega(s) e^{\Omega_u(s)} + \beta e^{-\Omega_u(s)} \omega(s) e^{\Omega_u(s)} \beta = -e^{\Omega_g(s)} (\eta(s) + \beta \eta(s) \beta) e^{-\Omega_g(s)} \equiv 0$$

(130)
That way a (hidden) correlation between the even and odd parts of the generator $\omega(s)$ of the beta-flow is revealed

$$\omega(s) = -e^{2\Omega_u(s)} (\beta \omega(s) \beta) e^{-2\Omega_u(s)}$$

(131)

In consequence of $\omega(s)$ being (in general) composed of even and odd terms,

$$\omega(s) = \omega_g(s) + \omega_u(s)$$

(132)

, then

$$\omega_g(s) + \omega_u(s) = e^{2\Omega_u(s)} (-\omega_g(s) + \omega_u(s)) e^{-2\Omega_u(s)}$$

(133)

$$= \exp (2\text{ad}_{\Omega_u(s)}) \circ (-\omega_g(s) + \omega_u(s))$$

, equivalently

$$\omega_g(s) = \tanh \left( \text{ad}_{\Omega_u(s)} \right) \circ \omega_u(s)$$

(134)

From this insight a useful relation connecting the generator $\eta(s)$ solely with the odd part $\omega_u(s)$ of the generator $\omega(s)$ emerges in the guise

$$-e^{\Omega_u(s)} \eta(s) e^{-\Omega_u(s)} = e^{-\Omega_u(s)} \omega(s) e^{\Omega_u(s)}$$

(135)

$$= \exp \left( -\text{ad}_{\Omega_u(s)} \right) \circ (\omega_g(s) + \omega_u(s))$$

$$= \exp \left( -\text{ad}_{\Omega_u(s)} \right) \left( \tanh \left( \text{ad}_{\Omega_u(s)} \right) + 1 \right) \circ \omega_u(s)$$

$$= \frac{1}{\cosh \left( \text{ad}_{\Omega_u(s)} \right)} \circ \omega_u(s)$$

Consequently the ODE (128) together with (132) leads to

$$\frac{d}{ds} \mathcal{V}(s) = \frac{d}{ds} \left( e^{\Omega_u(s)} e^{\Omega_g(s)} \right)$$

(136)

$$= \left( \frac{d}{ds} e^{\Omega_u(s)} \right) e^{\Omega_g(s)} + e^{\Omega_u(s)} \left( \frac{d}{ds} e^{\Omega_g(s)} \right)$$

$$= \omega(s) \left( e^{\Omega_u(s)} e^{\Omega_g(s)} \right)$$

$$= -e^{\Omega_u(s)} e^{\Omega_g(s)} \eta(s)$$

Employing the well known formula for the derivative of an exponential $e^{\Omega(s)}$ in case $[\Omega(s_1), \Omega(s_2)] \neq 0$, for instance [40], [41], now

$$\frac{d}{ds} e^{\Omega(s)} = \int_0^1 d\tau e^{\tau \Omega(s)} \frac{d}{ds} \Omega(s) e^{-\tau \Omega(s)} e^{\Omega(s)}$$

(137)

$$= \left( \int_0^1 d\tau e^{\tau \text{ad}_{\Omega(s)}} \circ \frac{d}{ds} \Omega(s) \right) e^{\Omega(s)}$$

$$= \left( \frac{\exp \left( \text{ad}_{\Omega(s)} \right) - 1}{\text{ad}_{\Omega(s)}} \circ \frac{d}{ds} \Omega(s) \right) e^{\Omega(s)}$$
Up next the ODE (136) along with (135) is readily shown to be equivalent to
\[-e^{\Omega_g(s)} \eta(s) e^{-\Omega_g(s)} = \frac{1}{\cosh(\text{ad}_{\Omega_u(s)})} \circ \omega_u(s) \]
\[= \frac{1 - \exp(-\text{ad}_{\Omega_u(s)})}{\text{ad}_{\Omega_u(s)}} \circ \frac{d}{ds} \Omega_u(s) + \frac{\exp(\text{ad}_{\Omega_u(s)}) - 1}{\text{ad}_{\Omega_g(s)}} \circ \frac{d}{ds} \Omega_g(s) \tag{138} \]
The left hand side in (138) being manifestly odd, the first term on the right hand side in (138) decomposes into even and odd parts
\[= \frac{1 - \exp(-\text{ad}_{\Omega_u(s)})}{\text{ad}_{\Omega_u(s)}} \circ \frac{d}{ds} \Omega_u(s) \tag{139} \]
\[= \left( \frac{1 - \cosh(\text{ad}_{\Omega_u(s)})}{\text{ad}_{\Omega_u(s)}} + \frac{\sinh(\text{ad}_{\Omega_u(s)})}{\text{ad}_{\Omega_u(s)}} \right) \circ \frac{d}{ds} \Omega_u(s) \]
\[= \frac{1 - \cosh(\text{ad}_{\Omega_u(s)})}{\text{ad}_{\Omega_u(s)}} \circ \frac{d}{ds} \Omega_u(s) + \frac{\sinh(\text{ad}_{\Omega_u(s)})}{\text{ad}_{\Omega_u(s)}} \circ \frac{d}{ds} \Omega_u(s) \]
, whereas the second term on the right hand side in (138) is manifestly even
\[= \frac{\exp(\text{ad}_{\Omega_u(s)}) - 1}{\text{ad}_{\Omega_g(s)}} \circ \frac{d}{ds} \Omega_g(s) = \sum_{n=0}^{\infty} \frac{1}{(n+1)!} \text{ad}_n(\Omega_g(s)) \circ \frac{d}{ds} \Omega_g(s) \tag{140} \]
A decomposition like (139) applies, because the commutator of an even operator with an even operator or else the commutator of an odd operator with an odd operator always results in an operator being even, whereas the commutator of an even operator with an odd operator and vice versa always results in an operator being odd.

Equating the even parts and the odd parts on either side of (138) regarded separately one obtains instead of (138) now two equations for \(\frac{d}{ds} \Omega_u(s)\) and \(\frac{d}{ds} \Omega_g(s)\)
\[\frac{\sinh(\text{ad}_{\Omega_u(s)})}{\text{ad}_{\Omega_u(s)}} \circ \frac{d}{ds} \Omega_u(s) = \frac{1}{\cosh(\text{ad}_{\Omega_u(s)})} \circ \omega_u(s) \tag{141} \]
\[\frac{1 - \cosh(\text{ad}_{\Omega_u(s)})}{\text{ad}_{\Omega_u(s)}} \circ \frac{d}{ds} \Omega_u(s) + \frac{\exp(\text{ad}_{\Omega_u(s)}) - 1}{\text{ad}_{\Omega_g(s)}} \circ \frac{d}{ds} \Omega_g(s) = 0 \tag{142} \]
Obviously, the first equation (141) directly determines \(\frac{d}{ds} \Omega_u(s)\), as it is decoupled from the equation for \(\frac{d}{ds} \Omega_g(s)\), whereas the determination of \(\frac{d}{ds} \Omega_g(s)\) with the second equation (142) requires prior knowledge of \(\frac{d}{ds} \Omega_u(s)\). Fortunately though, the determination of \(\Omega_g(s)\) is for the purpose of determining the Newton-Wigner Hamiltonian \(H^{(NW)}\) redundant, as the representation (126) reveals at one glance.
Solving finally (141) for \( \frac{d}{ds} \Omega_{u} (s) \) an equivalent ODE determining \( \Omega_{u} (s) \) is obtained

\[
\frac{d}{ds} \Omega_{u} (s) = \frac{2a d\Omega_{u}(s)}{\sinh (2a d\Omega_{u}(s))} \circ \omega_{u} (s) \tag{143}
\]

\( \Omega_{u} (0) = 0 \)

This being at first sight a scary nonlinear problem, in what follows it proves otherwise, noting that integration of (143) with respect to \( s \) leads to the integral equation

\[
\Omega_{u} (s) = \int_{0}^{s} ds' \frac{2a d\Omega_{u}(s')}{\sinh (2a d\Omega_{u}(s'))} \circ \omega_{u} (s') \tag{144}
\]

Provided the odd part \( \omega_{u} (s) \) of the generator \( \omega (s) \) of the beta-flow can be considered as being small, then that integral equation is amenable to a perturbative solution for the odd operator \( \Omega_{u} (s) \) by the method of Picard iteration. Clearly, the described perturbative solution method is a close relative to the well known Magnus series expansion, for a comprehensive review see [41].

**XIV. PERTURBATION SERIES FOR GENERATOR \( \omega (s) \) OF BETA-FLOW**

Unfortunately, it is difficult to obtain for a general Dirac Hamiltonian (127) an expansion of the generator

\[
\omega (s) = \left[ \hat{H}^{(D)}, Z (s) \right] = \sum_{n=1}^{\infty} \kappa^{n} \omega^{(n)} (s) \tag{145}
\]

with regard to the parameter \( \kappa \), even though the exact solution \( Z (s) \) of the beta-flow has been obtained in (56). To find the perturbation terms \( \omega^{(n)} (s) \) in (145) it is convenient to consider the operators

\[
Q (s) = Z (s) \hat{H}^{(D)}
\]

\[
Q^\dagger (s) = \hat{H}^{(D)} Z (s)
\]

, so that

\[
\omega (s) = Q^\dagger (s) - Q (s) \tag{147}
\]

From the beta-flow (55) we readily confirm that \( Q (s) \) solves the ODE

\[
\frac{1}{2} \frac{d}{ds} Q (s) = \hat{H}^{(D)} \hat{H}^{(D)} - Q (s) Q (s) \tag{148}
\]

\[
Q (0) = \beta \hat{H}^{(D)} = 1_{4 \times 4} + \kappa \beta \hat{O} + \kappa^{2} \beta \hat{E}
\]
Now a perturbation series expansion of the solution \( Q(s) \) to this ODE (148) is searched for in the guise

\[
Q(s) = 1_{4 \times 4} + \sum_{n=1}^{\infty} \kappa^n Q^{(n)}(s) \tag{149}
\]

Once the operators \( Q^{(n)}(s) \) are found, then

\[
\omega(s) = \sum_{n=1}^{\infty} \kappa^n \omega^{(n)}(s) \tag{150}
\]

\[
\omega^{(n)}(s) = (Q^{(n)}(s))^\dagger - Q^{(n)}(s)
\]

Insertion of the ansatz (149) into (148) gives

\[
\frac{d}{ds}Q(s) = \kappa \frac{d}{ds}Q^{(1)}(s) + \sum_{n=2}^{\infty} \kappa^n \frac{d}{ds}Q^{(n)}(s)
\]

, and minding

\[
\hat{\mathcal{O}} \beta = -\beta \hat{\mathcal{O}} \tag{151}
\]

\[
\hat{\mathcal{E}} \beta = \beta \hat{\mathcal{E}}
\]

\[
\beta \beta = 1_{4 \times 4}
\]

the inhomogenous term in the ODE (148) reads

\[
\hat{H}^{(D)} \hat{H}^{(D)} = \left( \beta + \kappa \hat{\mathcal{O}} + \kappa^2 \hat{\mathcal{E}} \right)^2 = 1_{4 \times 4} + \kappa^2 \left( 2 \beta \hat{\mathcal{E}} + \hat{\mathcal{O}}^2 \right) + \kappa^3 \left( \hat{\mathcal{E}} \hat{\mathcal{O}} + \hat{\mathcal{O}} \hat{\mathcal{E}} \right) + \kappa^4 \hat{\mathcal{E}}^2
\]

\[
\equiv 1_{4 \times 4} + \sum_{n=2}^{\infty} \kappa^n R^{(n)}
\]

\[
R^{(2)} = 2 \beta \hat{\mathcal{E}} + \hat{\mathcal{O}}^2
\]

\[
R^{(3)} = \hat{\mathcal{E}} \hat{\mathcal{O}} + \hat{\mathcal{O}} \hat{\mathcal{E}}
\]

\[
R^{(4)} = \hat{\mathcal{E}}^2
\]

\[
n > 4
\]

\[
R^{(n)} = 0_{4 \times 4}
\]

, where as the quadratic term in (148) assumes the guise

\[
Q(s)Q(s) = 1_{4 \times 4} + 2\kappa Q^{(1)}(s) + \sum_{n=2}^{\infty} \kappa^n \left( 2Q^{(n)}(s) + \sum_{j=1}^{n-1} Q^{(j)}(s) Q^{(n-j)}(s) \right) \tag{153}
\]
Comparing coefficients of $\kappa^n$ for $n = 1, 2, 3, \ldots$ on either side of (148) then the following set of linear differential equations for the determination of the operators $Q^{(n)}(s)$ is obtained

\[
\begin{align*}
\frac{1}{2} \frac{d}{ds} Q^{(1)}(s) &= -2Q^{(1)}(s) \\
&\quad \quad n \geq 2 \\
\frac{1}{2} \frac{d}{ds} Q^{(n)}(s) &= -2Q^{(n)}(s) + R^{(n)} - \sum_{j=1}^{n-1} Q^{(j)}(s) Q^{(n-j)}(s)
\end{align*}
\]

To be consistent with the initial data posed at $s = 0$ in (148) it is required

\[
\begin{align*}
Q^{(1)}(0) &= \beta \tilde{O} \\
Q^{(2)}(0) &= \beta \tilde{E} \\
&\quad \quad \text{for } n > 2 \\
Q^{(n)}(0) &= 0_{4 \times 4}
\end{align*}
\]

so that

\[
Q(0) = 1_{4 \times 4} + \sum_{n=1}^{\infty} \kappa^n Q^{(n)}(0)
\]

The retained inhomogeneous linear differential equations (154) are readily integrated and enable now a recursive determination of the operators $Q^{(n)}(s)$ as follows

\[
\begin{align*}
Q^{(1)}(s) &= e^{-4s} \beta \tilde{O} \\
&\quad \quad n \geq 2 \\
Q^{(n)}(s) &= e^{-4s} Q^{(n)}(0) + 2 \int_0^s ds' e^{-4(s-s')} \left( R^{(n)} - \sum_{j=1}^{n-1} Q^{(j)}(s') Q^{(n-j)}(s') \right)
\end{align*}
\]

A straightforward analysis of this recursion up to and including the terms of fourth order $Q^{(4)}(s)$ leads on the basis of (150) to the following results

\[
\begin{align*}
\omega^{(1)}(s) &= -2e^{-4s} \beta \tilde{O} \\
\omega^{(2)}(s) &= 0_{4 \times 4} \\
\omega^{(3)}(s) &= -4e^{-4s} \left[ \tilde{O}, \tilde{E} \right] + \left( e^{-4s} \left( -\frac{1}{2} + 4s \right) + \frac{e^{-12s}}{2} \right) \beta \tilde{O}^3 \\
\omega^{(4)}(s) &= \left( e^{-4s} \left( -\frac{1}{2} + 2s \right) + \frac{e^{-8s}}{2} \right) \beta \left[ \tilde{O}, \left( \tilde{E} \tilde{O} + \tilde{O} \tilde{E} \right) \right]
\end{align*}
\]
The result for $\omega^{(5)}(s)$ is available in the complemental material [12].

Quite generally, the recursion (157) reveals the even-numbered terms $\omega^{(2n)}(s)$ are even operators whereas the odd-numbered terms $\omega^{(2n+1)}(s)$ are odd operators:

$$
\beta \omega^{(2n)}(s) \beta = \omega^{(2n)}(s) \quad (162)
$$

$$
\beta \omega^{(2n+1)}(s) \beta = -\omega^{(2n+1)}(s) \quad (163)
$$

As a result of this the series expansion (145) representing the generator $\omega(s)$ decomposes into

$$
\omega(s) = \omega_g(s) + \omega_u(s)
$$

$$
\omega_g(s) = \sum_{n=2}^{\infty} \kappa^{2n} \omega^{(2n)}(s) \quad (164)
$$

$$
\omega_u(s) = \sum_{n=0}^{\infty} \kappa^{2n+1} \omega^{(2n+1)}(s)
$$

Note that because $\omega^{(2)}(s) \equiv 0$ the series determining the even part $\omega_g(s)$ of the generator $\omega(s)$ is small of order $O(\kappa^4)$.

**XV. PERTURBATION SERIES FOR OPERATOR $\Omega_u(s)$**

With

$$
\omega_u(s) = \sum_{n=0}^{\infty} \kappa^{2n+1} \omega^{(2n+1)}(s) \quad (165)
$$

being odd it is natural adopting a corresponding approach for a perturbative series expansion of $\Omega_u(s)$

$$
\Omega_u(s) = \sum_{n=0}^{\infty} \kappa^{2n+1} \Omega^{(2n+1)}(s) \quad (166)
$$

Writing

$$
\frac{2z}{\sinh(2z)} = 1 - \frac{2}{3}z^2 + \frac{14}{45}z^4 - \frac{124}{945}z^6 + O(z^8) \quad (167)
$$

there follows in place of (144)

$$
\Omega_u(s) = \int_0^s ds' \left( 1 - \frac{2}{3} (\text{ad}_{\Omega_u(s')})^2 + \frac{14}{45} (\text{ad}_{\Omega_u(s')})^4 - \frac{124}{945} (\text{ad}_{\Omega_u(s')})^6 + O(\kappa^8) \right) \circ \omega_u(s') \quad (168)
$$
Inserting the series expansions (165) and (166) into (168) one finds in a straightforward manner comparing coefficients of $\kappa^{2n+1}$ on either side of (168) a recursion relation determining the searched for terms $\Omega^{(2n+1)}(s)$. Obviously the first order term being

$$\Omega^{(1)}(s) = \int_0^s ds' \omega^{(1)}(s') = -\frac{1 - e^{-4s}}{2} \beta \tilde{O}$$

(169)

, this immediately implies the vanishing of the commutator

$$[\Omega^{(1)}(s'), \omega^{(1)}(s')] = 0$$

(170)

Consequently all the commutator terms $(\text{ad}_{\Omega^{(n)}(s')})^{2n} \circ \omega_u(s')$ in (168) are at least small of order $O(\kappa^{2n+3})$. With that said the third order term is

$$\Omega^{(3)}(s) = \int_0^s ds' \omega^{(3)}(s')$$

$$= \left(-\frac{1}{4} + e^{-4s} \left(\frac{1}{4} + s\right)\right) \left\{ \tilde{O}, \tilde{E} \right\} + \left(\frac{1}{6} - e^{-4s} \left(\frac{1}{8} + s\right) - \frac{e^{-12s}}{24}\right) \beta \tilde{O}^3$$

(171)

, whereas the fifth-order term is then determined by

$$\Omega^{(5)}(s) = \begin{cases} \int_0^s ds' \omega^{(5)}(s') \\ -\frac{2}{3} \int_0^s ds' \left[ \Omega^{(1)}(s'), \left[ \Omega^{(3)}(s'), \omega^{(1)}(s') \right] \right] + \left[ \Omega^{(1)}(s'), \left[ \Omega^{(1)}(s'), \omega^{(3)}(s') \right] \right] \end{cases}$$

(172)

An explicit evaluation of (172) is given in [12]. As we show in the ensuing, $\Omega^{(5)}(s)$ will appear in the calculations for the first time if the expansion of \( \hat{H}^{(D)} \) according to the lines indicated in (126) aims at an accuracy better than $\kappa^6$.

Note we did not adress the issue of the convergence of the Magnus-type expansion (166). Guided by physical intuition, with operators $\tilde{E}$ and $\tilde{O}$ assigned to a Dirac Hamiltonian in external potentials like in (12), the described expansion method is conjectured being convergent for all electric field strengths $\mathcal{E} = \left\| \frac{i}{\hbar} \left[ \tilde{O}, \tilde{E} \right] \right\|$ vastly below the Schwinger critical field $\mathcal{E}_S = \frac{m |e| c^2}{\lambda} \simeq 1.3 \times 10^{18} \left[ \frac{m}{m} \right]$. Perhaps one could find along the lines discussed in [41] a sharp estimate for the radius of convergence of that expansion (166), establishing that way, for instance, a stability criterion for the existence of the Newton-Wigner Hamiltonian of the relativistic electron in the presence of strong electrostatic fields.
XVI. THE RELATIVISTIC CORRECTIONS TO THE SCHRÖDINGER PAULI HAMILTONIAN $H^{(SP)}$ AS A SERIES PROGRESSING IN POWERS OF $\frac{v^2}{c^2}$

The remaining task is now to evaluate the afore given explicit representation (126) for the Newton-Wigner Hamiltonian as a series of iterated commutators by inserting the obtained series expansion for $\Omega_u(s)$ in (166) and to find that way the searched for perturbative terms $\Omega^{(2n+1)}(s)$. Let us agree in the ensuing on abbreviating the limiting value of the operator $\Omega_u(s)$ for $s \to \infty$ as

$$\Omega_u(\infty) \equiv \Omega_u = \kappa \Omega^{(1)} + \kappa^3 \Omega^{(3)} + \kappa^5 \Omega^{(5)} + ...$$

(173)

, whereby according to (169), (171), (172) the terms $\Omega^{(2n+1)} = \Omega^{(2n+1)}(\infty)$ are given by

$$\Omega^{(1)} = -\frac{1}{2} \beta \tilde{O}$$

$$\Omega^{(3)} = \frac{1}{6} \beta \tilde{O}^3 - \frac{1}{4} [\tilde{O}, \tilde{E}]$$

$$\Omega^{(5)} = -\frac{1}{10} \beta \tilde{O}^5 + \frac{1}{9} [\tilde{O}^3, \tilde{E}] + \frac{5}{144} [\tilde{O}, [\tilde{O}, [\tilde{O}, \tilde{E}]]] - \frac{1}{8} \beta [[[\tilde{O}, \tilde{E}], \tilde{E}]]$$

, and so on.

Restricting the expansion of $H^{(NW)}$ to accuracy $O(\kappa^8)$ it follows directly from (126)

$$\tilde{H}^{(NW)} = \begin{cases} 
\left(\beta + \kappa^2 \tilde{E}\right) \\
+\frac{1}{7} (\text{ad}_{\Omega_u})^2 \circ \left(\beta + \kappa^2 \tilde{E}\right) + \frac{1}{21} (\text{ad}_{\Omega_u})^4 \circ \left(\beta + \kappa^2 \tilde{E}\right) + \frac{1}{720} (\text{ad}_{\Omega_u})^6 \circ \left(\beta + \kappa^2 \tilde{E}\right) \\
- (\text{ad}_{\Omega_u}) \circ \kappa \tilde{O} - \frac{1}{6} (\text{ad}_{\Omega_u})^3 \circ \kappa \tilde{O} - \frac{1}{120} (\text{ad}_{\Omega_u})^5 \circ \kappa \tilde{O} \\
+ O(\kappa^8)
\end{cases}$$

(175)

At first sight the indicated accuracy $O(\kappa^8)$ holds true with the operator $\Omega_u$ being expanded up to and including the fifth order term $\Omega^{(5)}$, because with the expansion

$$\text{ad}_{\Omega_u} \circ \mathcal{F} = \sum_{j=0}^{\infty} \kappa^{2j+1} \text{ad}_{\Omega^{(2j+1)}} \circ \mathcal{F}$$

(176)
then

\[
(ad_{\Omega_n})^6 \circ \beta = \kappa^6 \left(ad_{\Omega(1)}\right)^6 \circ \beta + O(\kappa^8) \quad (177)
\]

\[
(ad_{\Omega_n(\infty)})^5 \circ \left(\kappa\bar{O}\right) = \kappa^6 \left(ad_{\Omega(1)}\right)^5 \circ \bar{O} + O(\kappa^8)
\]

\[
(ad_{\Omega_n})^4 \circ \left(\kappa^2\bar{E}\right) = \kappa^6 \left(ad_{\Omega(1)}\right)^4 \circ \bar{E} + O(\kappa^8)
\]

Yet the commutator terms at order \(\kappa^{2n}\) in the expansion (175) involving the operators \(\Omega^{(2n-1)}\)

\textit{cancel} for \(n \geq 2\), because of the identity

\[
\frac{1}{2}ad_{\Omega(1)} \circ ad_{\Omega^{(2n-1)}} \circ \beta + \frac{1}{2}ad_{\Omega^{(2n-1)}} \circ ad_{\Omega(1)} \circ \beta = ad_{\Omega^{(2n-1)}} \circ \bar{O} \quad (178)
\]

This is fortunate, as it implies, that in order to achieve accuracy \(O(\kappa^{2n})\) for \(n \geq 2\) only the operators \(\Omega^{(1)}, \Omega^{(3)}, \ldots, \Omega^{(2n-3)}\) are required! So we obtain from (175) now the following expansion for the (scaled) Newton-Wigner Hamiltonian in the guise (here we set \(\kappa = 1\), as no book keeping is required anymore)

\[
\tilde{H}^{(NW)} = \beta + \tilde{h}^{(2)} + \tilde{h}^{(4)} + \tilde{h}^{(6)} + \ldots 
\]

(179)

whereas

\[
\tilde{h}^{(2)} = \bar{E} + \frac{1}{2} \left[\Omega^{(1)}, \left[\Omega^{(1)}, \beta\right]\right] - \left[\Omega^{(1)}, \bar{O}\right] 
\]

(180)

\[
\tilde{h}^{(4)} = \left( \begin{array}{c}
\frac{1}{24} \left[\Omega^{(1)}, \left[\Omega^{(1)}, \left[\Omega^{(1)}, \left[\Omega^{(1)}, \beta\right]\right]\right]\right] \\
\frac{1}{2} \left[\Omega^{(1)}, \left[\Omega^{(1)}, \bar{E}\right]\right] \\
-\frac{1}{6} \left[\Omega^{(1)}, \left[\Omega^{(1)}, \left[\Omega^{(1)}, \bar{O}\right]\right]\right]
\end{array} \right) 
\]

(181)
A straightforward analysis \cite{12} of these expressions leads to

\[
\tilde{h}^{(2)} = \tilde{\mathcal{E}} + \frac{1}{2} \beta \tilde{\mathcal{O}}^2
\]

(183)

\[
\tilde{h}^{(4)} = -\frac{1}{8} \beta \tilde{\mathcal{O}}^4 - \frac{1}{8} \left[ \tilde{\mathcal{O}}, \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right] \right]
\]

(184)

\[
\tilde{h}^{(6)} = \begin{cases}
\frac{1}{16} \beta \tilde{\mathcal{O}}^6 \\
\frac{1}{32} \left[ \tilde{\mathcal{O}}^3, \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right] \right] + \frac{1}{64} \left[ \tilde{\mathcal{O}}, \left( \mathcal{O}^2 \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right] + \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right] \mathcal{O}^2 \right) \right] \\
+ \frac{1}{128} \left[ \tilde{\mathcal{O}}, \left[ \tilde{\mathcal{O}}, \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right] \right] \right] \\
+ \frac{1}{16} \beta \left( \tilde{\mathcal{O}} \left[ \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right], \tilde{\mathcal{E}} \right] \right) + \left[ \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right], \tilde{\mathcal{E}} \right] \tilde{\mathcal{O}} \right)
\end{cases}
\]

(185)

The term \(\tilde{h}^{(2)}\) in (183) is the Hamiltonian of Schrödinger Pauli quantum mechanics (scaled units). The term \(\tilde{h}^{(4)}\) in (184) coincides with the standard outcome for the relativistic correction to the kinetic energy, the Darwin term and the spin-orbit interaction term.
with the (static) external electric field, in agreement with the (laborious) step-by-step FW-
transformation method [2].

Beyond order $\kappa^4$ results obtained by the FW-transformation method are not energy-
separating. This has been realized already early on by Eriksen and Kolsrud [14]. An
additional unitary transformation is required to generate suitable correction terms, so that
the results obtained then coincide with results obtained by the Eriksen method [5]. A general
scheme that provides for the original FW-transformation to every order $\kappa^{2n}$ the required
correction terms, so that it coincides with the result of the (tedious) Eriksen transformation
method expanded to that same order $\kappa^{2n}$, has been developed by Silenko [37].

It should be emphasized that our result for $\tilde{h}^{(6)}$ in (185) is by construction energy-
separating. The result is in accord with results obtained by Silenko’s correction scheme
[37] applied to the original FW-transformation, and it also coincides with the table pro-
vided by deVries and Jonker [34], who obtained (though in a less practicable guise) their
expansion in powers of $\kappa = \frac{v}{c}$ with the Pauli-Achieser-Berestezki elimination method (using
computer algebra) and provided a proof of equivalence of their approach with the unitary
transformation method of Eriksen.

The introduced expansion method, see (126) together with (144), constitutes the central
result of this article. It fully implements a convenient energy-separating scheme to recon-
struct the expansion in powers of $\frac{v}{c}$ for the Newton-Wigner Hamiltonian of the relativistic
electron moving in static external potentials.

**XVII. HAMILTONIAN FLOW EQUATIONS FOR TIME-DEPENDENT ELECTRO-
MAGNETIC FIELDS**

We consider now a (scaled) time-dependent Dirac Hamiltonian, composed of even and
odd parts

$$\tilde{H}^{(D)}(t) = \beta + \tilde{E}(t) + \tilde{O}(t)$$

(186)

, agreeing in what follows to choose $\beta$ and $\alpha_b$ in Dirac-Pauli representation, always minding
$\beta$ being then a diagonal matrix (for details and a discussion of other unitary equivalent repre-
sentations see the useful appendix A-2 in ref. [19]). For instance, taking into account external
(c-number valued) electromagnetic fields with prescribed (parametric) time-dependence,

\[ \mathcal{E}_b (\mathbf{r}, t) = -\frac{\partial \Phi (\mathbf{r}, t)}{\partial r_b} - \frac{\partial A_b (\mathbf{r}, t)}{\partial t} \]  

\[ \mathcal{B}_a (\mathbf{r}, t) = \varepsilon_{abc} \frac{\partial}{\partial r_b} A_c (\mathbf{r}, t) \]  

(187)

\[ \mathcal{B}_a (\mathbf{r}, t) = \varepsilon_{abc} \frac{\partial}{\partial r_b} A_c (\mathbf{r}, t) \]

then the even and odd operators in (186) are, respectively

\[ \tilde{\mathcal{E}} (t) = \frac{q_e}{mc^2} \Phi (\mathbf{x}, t) \mathbf{1}_{4 \times 4} \]  

(188)

\[ \tilde{\mathcal{O}} (t) = \alpha_b \frac{\Pi_b}{mc} \]  

(189)

\[ \Pi_b \equiv \Pi_b (\mathbf{p}, \mathbf{x}, t) = \mathbf{p}_b - q_e A_b (\mathbf{x}, t) \]

In the ensuing a flow equation based scheme is searched for to find a time-dependent unitary transformation \( U (t, s) \) of the four-component Dirac Amplitude \( \Psi_{\mu}^{(D)} (\mathbf{r}, t) \) that strives for \( s \to \infty \) to an amplitude

\[ \Psi_{\mu}^{(U)} (\mathbf{r}, t) = U_{\mu, \mu'} (t, \infty) \Psi_{\mu'}^{(D)} (\mathbf{r}, t) \]

in the guise (28), so that also in the presence of spatiotemporal electromagnetic fields separate equations of motion govern the time development of the two-component amplitudes \( \psi_\sigma (\mathbf{r}, t) \) and \( \chi_\sigma (\mathbf{r}, t) \) for all times.

Specifically, if at time \( t = 0 \) there holds \( \Psi_{\mu}^{(U)} (\mathbf{r}, 0) = 0 \) for \( \mu = 3, 4 \) then at all later times \( t > 0 \) it ought to be as well \( \Psi_{\mu}^{(U)} (\mathbf{r}, t) = 0 \) for \( \mu = 3, 4 \). Ditto, if at time \( t = 0 \) there holds \( \Psi_{\mu}^{(U)} (\mathbf{r}, 0) = 0 \) for \( \mu = 1, 2 \) then at all later times \( t > 0 \) it ought to be as well \( \Psi_{\mu}^{(U)} (\mathbf{r}, t) = 0 \) for \( \mu = 1, 2 \).

This not being the only distinctive feature of the unitary transformation \( U (t, \infty) \) it is concurrently required that returning to the special case of static fields the unitary transformation \( U (t, s) \) should coincide with the afore obtained unitary transformation (77), the latter converging for \( s \to \infty \) to the unitary transformation \( T \) in (92) equivalent to the Eriksen transformation.

Now choosing as initial value of the flow at \( s = 0 \) the (scaled) time dependent Dirac Hamiltonian \( \tilde{\mathcal{H}}^{(D)} (t) \) defined in (186), a unitary transformed time-dependent Hamiltonian \( \tilde{\mathcal{H}}^{(U)} (s, t) \) arises, that governs the time evolution of the unitary transformed Dirac amplitude

\[ \Psi_{\mu}^{(U)} (\mathbf{r}, t; s) = U_{\mu, \mu'} (t, s) \Psi_{\mu'}^{(D)} (\mathbf{r}, t; s) \]
at fixed value $s$ according to
\[
\tilde{H}^{(U)}(t, s) = U(t, s) \circ \left( \tilde{H}^{(D)}(t) - i\hat{\partial}_t \right) \circ U^\dagger(t, s) + i\hat{\partial}_t \tag{190}
\]
so that instead of
\[
i\frac{\hbar}{mc^2} \frac{\partial}{\partial t} \Psi^\mu(r, t) = \tilde{H}^{(D)}_{\mu,\mu'}(t) \Psi^\mu_{\mu'}(r, t) \tag{191}
\]
we have now
\[
i\frac{\hbar}{mc^2} \frac{\partial}{\partial t} \Psi^\mu_U(r, t; s) = \tilde{H}^{(U)}_{\mu,\mu'}(t, s) \Psi^\mu_{\mu'}(r, t; s) \tag{192}
\]
\[
\Psi^\mu_U(r, t; 0) = \Psi^\mu_{(D)}(r, t) \tag{193}
\]
For convenience here we introduced the symbol $\hat{\partial}_t$ to denote a \textit{scaled} time derivative \textit{operator} so that
\[
\left[ \hat{\partial}_t, U^\dagger(t, s) \right] = \frac{\hbar}{mc^2} \frac{\partial}{\partial t} U^\dagger(t, s) \tag{193}
\]
Note the unitary transformation $U(t, s)$ depends on the flow parameter $s$ and on time $t$ in consequence of the time dependence of the initial data of the flow at $s = 0$ given by
\[
U(t, 0) = 1_{4 \times 4} \tag{194}
\]
\[
\tilde{H}^{(U)}(t, 0) = \tilde{H}^{(D)}(t) \tag{195}
\]
Because the time derivative \textit{operator} $i\hat{\partial}_t$ in the Dirac equation \textit{(191)} necessarily gets affected too by any time-dependent unitary transformation, as emphasized in \textit{[2]}, at first sight the method(s) described in the previous sections for static external fields are not likely to apply.

Progress comes introducing the \textit{operator}
\[
K(t, s) \equiv \tilde{H}^{(U)}(t, s) - i\hat{\partial}_t = U(t, s) \left( \tilde{H}^{(D)}(t) - i\hat{\partial}_t \right) U^\dagger(t, s) \tag{196}
\]
Given a suitable generator $\eta(t, s) = -\eta^\dagger(t, s)$ of the Hamiltonian flow then the associated unitary transformation is determined by
\[
\frac{\partial}{\partial s} U(t, s) = \eta(t, s) U(t, s) \tag{196}
\]
\[
U(t, 0) = 1_{4 \times 4}
\]
, and with that said the ODE determining $K(t, s)$ and taking into account the initial data \textit{(194)} reads
\[
\frac{\partial}{\partial s} K(t, s) = [\eta(t, s), K(t, s)] \tag{197}
\]
\[
K(t, 0) = \tilde{H}^{(D)}(t) - i\hat{\partial}_t
\]
A specific flow equation striving towards a *time-dependent* Newton-Wigner representation, that we now introduce in full analogy to the previous (static) flow equation approach (96), employs as a time-dependent generator

\[ \eta(t, s) = [\beta, K(t, s)] \] (198)

The proof of the wanted property \( K(t, \infty) \) being even (block-diagonal), i.e.

\[ \lim_{s \to \infty} \eta(t, s) = 0_{4 \times 4} \] (199)

is readily transferred from it’s static prefiguration adjusting the functional (3) and it’s derivative (5) to the time-dependent case.

Combining now the generator (198) with (197) thereby emerges the time-dependent flow equation

\[
\frac{\partial}{\partial s} K(t, s) = [[\beta, K(t, s)], K(t, s)] \\
K(t, 0) = \beta + \hat{O}(t) + \hat{E}(t) - i\hat{\partial}_t
\] (200)

\( K(t, 0) = \beta + \hat{O}(t) + \hat{E}(t) - i\hat{\partial}_t \)

, with the limiting value \( K(t, \infty) \) of that flow for \( s \to \infty \) by construction being even, i.e. \( [\beta, K(t, \infty)] = 0_{4 \times 4} \).

Introducing a splitting of the operator \( K(t, s) \) into an *even* operator \( K_g(t, s) \) and an *odd* operator \( K_u(t, s) \),

\[
K(t, s) = \frac{1}{2} (K(t, s) + \beta K(t, s) \beta) + \frac{1}{2} (K(t, s) - \beta K(t, s) \beta) \\
\equiv K_g(t, s) + K_u(t, s)
\] (201)

\[ \beta K_g(t, s) = K_g(t, s) \beta \]
\[ \beta K_u(t, s) = -K_u(t, s) \beta \]

, the generator \( \eta(t, s) \) of the flow is indeed the generalization of the time-independent generator used by Bylev and Pirner [11] to the time-dependent case:

\[ \eta(t, s) = [\beta, K(t, s)] = 2\beta K_u(t, s) \] (202)

Consequently the flow equation (200) determining the operator \( K(t, s) \) is equivalent to two coupled equations determining \( K_g(t, s) \) and \( K_u(t, s) \):

\[
\frac{d}{ds} K_g(t, s) = [[\beta, K_u(t, s)], K_u(t, s)] = 4\beta K_u(t, s) K_u(t, s) \\
\frac{d}{ds} K_u(t, s) = [[\beta, K_u(t, s)], K_g(t, s)] = 2\beta [K_u(t, s), K_g(t, s)]
\] (203)
\[ K_g (t, 0) = \beta + \tilde{E} (t) - i \hat{\partial}_t \]
\[ K_u (t, 0) = \tilde{O} (t) \]  

In general we don’t expect to find an exact solution to (200). But if we restrict to the nonrelativistic sector and to weak field strengths (far below the Schwinger critical field) with slow time-dependence compared with the fast time scale set by \( \frac{mc}{\hbar} \), a series expansion of the sought solutions \( K_g (t, s) \) and \( K_u (t, s) \) progressing in powers of the small parameter \( \kappa = \frac{v}{c} \) is adequate:

\[ K_g (t, s) = \beta + \sum_{j=1}^{\infty} \kappa^{2j} K^{(2j)} (t, s) \]  
\[ K_u (t, s) = \sum_{j=0}^{\infty} \kappa^{2j+1} K^{(2j+1)} (t, s) \]

In view of our aim obtaining from the Dirac Hamiltonian the nonrelativistic Schrödinger-Pauli quantum mechanics together with the relativistic corrections progressing in powers of \( \kappa \) now for a time-dependent Dirac Hamiltonian here we rank the term \( \tilde{E} (t) - i \hat{\partial}_t \) on equal footing with \( \tilde{O} (t) \tilde{O} (t) \). Of course, if strong(er) electric fields should be considered, like during the passage of an electron near by an atomic nucleus in a scattering experiment, then a ranking of \( \tilde{E} (t) - i \hat{\partial}_t \) on equal footing with \( \tilde{O} (t) \) should be preferable.

For consistency with (204) the initial data of those series elements \( K^{(j)} (t, s) \) at \( s = 0 \) are

\[ K^{(1)} (t, 0) = \tilde{O} (t) \]  
\[ K^{(2)} (t, 0) = \tilde{E} (t) - i \hat{\partial}_t \]  
\[ j \geq 3 \]  
\[ K^{(j)} (t, 0) = 0_{4 \times 4} \]

Insertion of the series representations (205) into the non linear differential equations (203) a linear system of coupled ordinary differential equations emerges enabling the recursive determination of the sequence of operators \( K^{(j)} (0, t) \) in full analogy to the afore addressed (simpler) case of a time-independent Hamiltonian [11]. That way with the prescribed initial
data at $s = 0$ the recursion relation obtained reads

\begin{equation}
K^{(2n)}(t, s) = K^{(2n)}(t, 0) + 4\beta \sum_{j=0}^{n-1} \int_0^s ds' K^{(2j+1)}(t, s') K^{(2n-2j-1)}(t, s')
\end{equation}

\begin{equation}
K^{(2n+1)}(t, s) = e^{-4s} K^{(2n+1)}(t, 0) + 2\beta \sum_{j=0}^{n-1} \int_0^s ds' e^{-4(s-s')} \left[ K^{(2j+1)}(t, s'), K^{(2n-2j)}(t, s') \right]
\end{equation}

All odd numbered terms $K^{(2n+1)}$ manifestly vanishing in the limit $s \to \infty$ the searched for unitary transformed operator $K(t, s)$ emerges in the limit $s \to \infty$ as a series of terms progressing in powers of $\kappa^2$ given by

\begin{equation}
K(t, \infty) = \beta + \sum_{j=1}^{\infty} \kappa^{2j} K^{(2j)}(t, \infty)
\end{equation}

\begin{equation}
\tilde{H}^{(U)}(t, \infty) = i \hat{\partial}_t + K(t, \infty)
\end{equation}

For convenience let us adopt compact notation

\begin{equation}
\tilde{\mathcal{F}} = \tilde{\mathcal{E}}(t) - i \hat{\partial}_t
\end{equation}

\begin{equation}
\tilde{O} = \tilde{O}(t)
\end{equation}

\begin{equation}
\tilde{\mathcal{E}} = \tilde{\mathcal{E}}(t)
\end{equation}

With the details of the calculations all recorded in [12], let us summarize our results obtained from straightforward perturbation theory up to and including the sixth order terms $\kappa^6$:

\begin{equation}
\tilde{H}^{(U)}(t, \infty) = \beta + \kappa^2 \tilde{h}^{(U, 2)}(t) + \kappa^4 \tilde{h}^{(U, 4)}(t) + \kappa^6 \tilde{h}^{(U, 6)}(t) + \ldots
\end{equation}

whereas (scaled units)

\begin{equation}
\tilde{h}^{(U, 2)}(t) = \tilde{\mathcal{E}} + \beta \frac{\tilde{O}^2}{2}
\end{equation}

\begin{equation}
\tilde{h}^{(U, 4)}(t) = -\frac{1}{8} \beta \tilde{O}^4 - \frac{1}{8} \left[ \tilde{O}, \left[ \tilde{O}, \tilde{\mathcal{F}} \right] \right]
\end{equation}

\begin{equation}
\tilde{h}^{(U, 6)}(t) = \begin{cases}
+\frac{1}{16} \beta \tilde{O}^6 + \frac{1}{16} \beta \left( \tilde{O}^2 \tilde{\mathcal{F}}^2 + \tilde{\mathcal{F}}^2 \tilde{O}^2 - 2 \tilde{O} \tilde{\mathcal{F}} \tilde{O} \tilde{\mathcal{F}} - 2 \tilde{\mathcal{F}} \tilde{O} \tilde{\mathcal{F}} \tilde{O} + 2 \tilde{O} \tilde{\mathcal{F}}^2 \tilde{O} \right) \\
+\frac{7}{128} \left( \tilde{\mathcal{O}}^4 \tilde{\mathcal{F}} + \tilde{\mathcal{F}} \tilde{\mathcal{O}}^4 \right) - \frac{3}{32} \left( \tilde{\mathcal{O}}^3 \tilde{\mathcal{F}} \tilde{O} + \tilde{\mathcal{O}} \tilde{\mathcal{F}} \tilde{O} \tilde{\mathcal{F}} \right) + \frac{5}{64} \tilde{\mathcal{O}}^2 \tilde{\mathcal{F}} \tilde{O}^2 \\
-\frac{1}{32} \beta \left[ \tilde{\mathcal{F}}, \left[ \tilde{\mathcal{F}}, \tilde{O}^2 \right] \right] + \frac{1}{64} \left[ \tilde{O}^2, \left[ \tilde{O}^2, \tilde{\mathcal{F}} \right] \right]
\end{cases}
\end{equation}
The term $\tilde{h}^{(U,2)}(t)$ is the (expected) nonrelativistic Hamiltonian of Schrödinger-Pauli quantum mechanics in the presence of time-dependent electromagnetic fields.

The fourth order term $\tilde{h}^{(U,4)}(t)$ adds to $h^{(U,2)}(t)$ the leading order relativistic corrections. It comprises, besides the correction to the kinetic energy $-\frac{1}{8}\beta\tilde{O}^4$, the Darwin term and the spin-orbit interaction, both terms encoded in the double commutator $-\frac{1}{8} [\tilde{O}, [\tilde{O}, \tilde{F}]]$, but now with the time-dependent total electric field (longitudinal and transversal). This is readily seen evaluating first, with $\tilde{O}$ and $\tilde{E}$ as given in (189), (188), the commutator

$$[\tilde{O}, [\tilde{O}, \tilde{F}]] = [\tilde{\Pi}_b, (\tilde{E} - i\tilde{\partial}_b)]$$

$$= \left(\frac{1}{mc}\right) \left(\frac{\hbar q_e}{mc^2}\right) i \left(-\frac{\partial \Phi(r, t)}{\partial r_b} - \frac{\partial A_b(r, t)}{\partial t}\right) \alpha_b$$

$$= \left(\frac{1}{mc^2 mc}\right) i\tilde{E}_b(r, t) \alpha_b$$

$$\equiv i\tilde{\partial}_b (r, t) \alpha_b$$

, whereby $\tilde{\partial}_b (r, t)$ denotes now the (scaled) total electric field including both contributions, longitudinal and transversal. Subsequently one finds

$$[\tilde{O}, [\tilde{O}, \tilde{F}]] = [\tilde{\Pi}_a \alpha_a, i\tilde{\partial}_b (r, t) \alpha_b]$$

$$= \frac{1}{2} \left([\tilde{\Pi}_a, i\tilde{\partial}_b] 2\delta_{ab} \mathbb{1}_{4 \times 4} + i \left(\tilde{\Pi}_a \tilde{\partial}_b + \tilde{\partial}_b \tilde{\Pi}_a\right) 2i\varepsilon_{ab\nu} \sigma_\nu\right)$$

$$= \frac{1}{mc} \left(\frac{1}{mc} \frac{\hbar q_e}{mc^2}\right) \left(\hbar \text{div}\tilde{E} - \tilde{\Pi} \wedge \tilde{E} + \tilde{E} \wedge \tilde{\Pi}\right)_{\nu} \sigma_\nu$$

Note the contribution of the transversal electric field to the spin-orbit interaction is missed out in the flow equation approach [11], as it applies only to static external potentials.

The term $\tilde{h}^{(U,6)}(t)$ represents the corrections of order $\kappa^6$ as obtained by the above presented Hamiltonian flow equation method. This term we stated here for clarification and for comparison only. Specializing to time-independent fields, then in all commutator terms we have $\tilde{F} \equiv \tilde{E}$, and comparing with our afore obtained energy-separating result (185) there is indeed a discrepancy

$$\tilde{h}^{(U,6)} = \tilde{h}^{(6)} - \frac{1}{32} \beta [\tilde{E}, [\tilde{E}, \tilde{O}^2]] + \frac{1}{64} \left[\tilde{\partial}^2, \left[\tilde{\partial}^2, \tilde{E}\right]\right]$$

$$= \frac{1}{32} \left[\beta [\tilde{E}, \tilde{O}^2], \tilde{h}^{(2)}\right]$$

That the established step-by-step Foldy-Wouthuysen method actually disagrees in the sixth order term $\tilde{h}^{(FW,6)}$ with results obtained by the (tedious) perturbative Eriksen method, has
been discovered already early on for minimal coupling to static fields \[ \text{[14]} \). So it comes as no surprise learning that our results obtained for \( \tilde{H}^{(U)}(t, \infty) \) with the afore discussed time-dependent Hamiltonian flow equation method \[ \text{[200]} \), if expanded beyond order \( \kappa^4 \), now disagree as well with the afore obtained contribution \[ \text{[185]} \) to the Newton-Wigner Hamiltonian.

As regards the additional discrepancy \( \tilde{h}^{(FW,6)} \neq \tilde{h}^{(U,6)} \), this is reflecting merely the afore mentioned ambiguity \[ \text{[33]} \) regarding unitary transformations \( U \) and also \( NU \) both transforming the Dirac Hamiltonian to a block-diagonal guise.

**XVIII. CONSTRUCTION OF THE NEWTON-WIGNER HAMILTONIAN FOR A DIRAC FERMION WITH MINIMAL COUPLING TO TIME-DEPENDENT ELECTROMAGNETIC FIELDS**

In this section we first introduce a generalization of the afore discussed static beta-flow equation method \[ \text{[200]} \) in order to derive now the time-dependent Newton-Wigner Hamiltonian associated with a time-dependent Dirac Hamiltonian. The proposition being, that all is required to lift the previous result for static fields \[ \text{[126]} \) now to time-dependent fields, lies in the replacement \[ \text{[14]} \]

\[
\tilde{E} \to \tilde{F}(t) = \tilde{E}(t) - i\hat{\partial}_t
\]

in all commutators defining the Newton-Wigner Hamiltonian \[ \text{[126]} \), as generated with the expansions \[ \text{[126]} \) and \[ \text{[144]} \), respectively \[ \text{[168]} \). To provide a proof we introduce to this end now a time-dependent beta-flow

\[
\frac{\partial}{\partial s}Z(t, s) = [\omega(t, s), Z(t, s)]
\]

\[
Z(t, 0) = \beta
\]

(214)

In contrast to the afore discussed (static) beta-flow in \[ \text{[13]} \) here we adopt the generator \( \omega(t, s) \) in such a way, that the operator

\[
\tilde{K}(t) = \tilde{H}^{(D)}(t) - i\hat{\partial}_t
\]

obeys to

\[
\left[ \tilde{K}(t), Z(t, \infty) \right] = 0_{4 \times 4}
\]

(216)
Along the line of reasoning presented afore in (4) a suitable antisymmetric generator of such a time-dependent beta-flow emerges as

$$\omega(t, s) = \left[ \tilde{K}(t), Z(t, s) \right]$$ (217)

Every bit said afore in the static case applies now in the time-dependent case with the operator $\tilde{K}(t)$ in place of $\tilde{H}(D)$. With that said the exact solution to (43) reads

$$Z(t, s) = W(t, s) \beta W^{-1}(t, s)$$ (218)

, whereas

$$W(t, s) = C(t, s) \beta + S(t, s)$$ (219)

$$C(t, s) = \cosh \left( 2s \tilde{K}(t) \right) = \cosh \left( 2s \sqrt{\tilde{K}(t) \tilde{K}(t)} \right)$$

$$S(t, s) = \sinh \left( 2s \tilde{K}(t) \right) = \frac{\tilde{K}(t)}{\sqrt{\tilde{K}(t) \tilde{K}(t)}} \sinh \left( 2s \sqrt{\tilde{K}(t) \tilde{K}(t)} \right)$$

As follows in reference to the exact solution (218) one readily confirms

$$Z(t, s) = Z^\dagger(t, s)$$ (220)

$$[\beta, (\beta Z(t, s) + Z(t, s) \beta)] = 0_{4 \times 4} = [[Z(t, s), (\beta Z(t, s) + Z(t, s) \beta)]]$$

$$Z(t, s) Z^\dagger(t, s) = Z^\dagger(t, s) Z(t, s)$$

$$Z(t, s) Z(t, s) = 1_{4 \times 4}$$

, thus validating the operator $Z(t, s)$ being unitary (and involutive as well). Furthermore the exact solution (218) has the limiting value

$$\lim_{s \to \infty} Z(t, s) = Z(t, \infty) = \frac{\tilde{K}(t)}{\sqrt{\tilde{K}(t) \tilde{K}(t)}}$$ (221)

In full analogy to the afore discussed time-independent case there follows, introducing the unitary operator

$$V(t, s) \equiv \frac{\beta + Z(t, s)}{\sqrt{(\beta + Z(t, s))^2} \beta}$$
And just like in the time-independent case there holds on the basis of the commutator relation stated in (220).

\[ V(t, s) V(t, s) = Z(t, s) \beta \] (223)

In view of the close analogy between the static case discussed afore in (VI) and the here treated time-dependent case, it seems natural there exists the solution \( K(t, s) \) to the (non-linear) Hamiltonian flow equation (200) with time-dependent generator (198) in the guise

\[ K(t, s) = V^\dagger(t, s) \tilde{K}(t) V(t, s) \] (224)

, with \( V(t, s) \) now a specific unitary transformation solving the initial value problem

\[ \frac{\partial}{\partial s} V(t, s) = \omega(t, s) V(t, s) \] (225)
\[ V(t, 0) = 1_{4\times4} \]

, and \( \omega(t, s) \) being the antisymmetric generator of the time-dependent beta-flow (43)

\[ \omega(t, s) = \left[ \tilde{K}(t), Z(t, s) \right] \] (226)

The validation of (224) follows readily directly from (225) and leads akin to the time-independent case (96) to

\[ \frac{\partial}{\partial s} K(t, s) = \left[ [\beta, K(t, s)], K(t, s) \right] \] (227)

, or else

\[ \frac{\partial}{\partial s} K(t, s) = [\eta(t, s), K(t, s)] \] (228)
\[ \eta(t, s) = [\beta, K(t, s)] \]
\[ K(t, 0) = \tilde{K}(t) \]

The flow equation obtained for \( K(t, s) \) this way coincides with the time-dependent flow (200), thus substantiating the assertion (224).

The now time-dependent generators, \( \eta(t, s) \) and \( \omega(t, s) \), with \( \eta(t, s) \) being odd and \( \omega(t, s) = \omega_u(t, s) + \omega_g(t, s) \) being decomposed into an even and an odd part (just like
in the time-independent case), are mutually connected by the same unitary transformation $V(t, s)$, i.e. once $\omega(t, s)$ is known, then $\eta(t, s)$ is known and vice versa

$$
\eta(t, s) = -V^*(t, s) \omega(t, s) V(t, s)
$$

(229)

Representing next, like before in the static case [XVI], the unitary transformation as

$$
V(t, s) = e^{\Omega_g(t, s)} e^{\Omega_u(t, s)}
$$

(230)

, with $\Omega_g(t, s)$ being even and $\Omega_u(t, s)$ being odd, then (229) implies

$$
e^{-\Omega_u(t, s)} \omega(t, s) e^{\Omega_u(t, s)} = -e^{\Omega_g(t, s)} \eta(t, s) e^{-\Omega_g(t, s)}
$$

This important fact engenders that everything said afore regarding the result for the perturbation expansion in the time-independent case, applies as well in the time-dependent case, so that we have in full analogy to the derivation of (144) now

$$
\Omega_u(t, s) = \int_0^s ds' \frac{2ad\Omega_u(t, s')}{\sinh(2ad\Omega_u(t, s'))} \circ \omega_u(t, s')
$$

(231)

Identifying the limiting value of the time-dependent flow determining $\tilde{H}^{(U)}(t, s)$ as

$$
\tilde{H}^{(U)}(t, \infty) - i\hat{\partial}_t \equiv K(t, \infty)
$$

(232)

$$
= \lim_{s \to \infty} V^*(t, s) K(t) V(t, s)
$$

$$
= \lim_{s \to \infty} e^{-\Omega_u(t, s)} e^{-\Omega_g(t, s)} K(t) e^{\Omega_g(t, s)} e^{\Omega_u(t, s)}
$$

, and because the limiting value $K(t, \infty)$ of the flow (228) obeys by construction to $[\beta, K(t, \infty)] = 0$, now the searched for time-dependent Newton-Wigner (NW) Hamiltonian arises in the guise

$$
\tilde{H}^{(NW)}(t) - i\hat{\partial}_t \equiv e^{+\Omega_g(t, \infty)} K(t, \infty) e^{-\Omega_g(t, \infty)}
$$

(233)

$$
= e^{-\Omega_u(t, \infty)} K(t) e^{\Omega_u(t, \infty)}
$$

$$
= e^{-\Omega_u(t, \infty)} \left( \beta + \tilde{\Omega}(t) + \tilde{E}(t) - i\hat{\partial}_t \right) e^{\Omega_u(t, \infty)}
$$

As the first line in (233) is manifestly even, we convert, like before in the static case [XVI], now the last line in (233) to the identical guise

$$
\tilde{H}^{(NW)}(t) = i\hat{\partial}_t + \cosh(ad\Omega_u(t, \infty)) \circ \left( \beta + \tilde{E}(t) - i\hat{\partial}_t \right) - \sinh(ad\Omega_u(t, \infty)) \circ \tilde{\Omega}(t)
$$

(234)

$$
= \beta + \tilde{E}(t) \left( \cosh(ad\Omega_u(t, \infty)) - 1 \right) \circ \left( \beta + \tilde{E}(t) - i\hat{\partial}_t \right) - \sinh(ad\Omega_u(t, \infty)) \circ \tilde{\Omega}(t)
$$
So in all commutators comprising in the static case a term \( \tilde{E} \), the transition to the time-dependent case is enabled making in the expansion (126), respectively in (183), (184), (185) and so on, the substitution

\[
\tilde{E} \rightarrow \tilde{F} (t) = \tilde{E} (t) - i\hat{\partial}_t
\]  

(235)

Note that the substitution rule (235) here arises out of the presented time-dependent generalization of the beta-flow striving to the limiting value (220), whereby the latter reduces in the stationary case to the energy-sign operator of the Dirac Hamiltonian. The substitution (235) has been established, on an observational basis though, already in [14], as it facilitates as well the calculational effort with the tedious original step by step FW-method significantly [37].

CONCLUSION

Proceeding from Brockett’s approach to continuous unitary transformations via flow equations with quadratic nonlinearity with a purpose-built generator \([\Gamma, H(s)]\) of the flow that strives for \( s \rightarrow \infty \) towards zero [9], the Hamiltonian flow considered by Bylev and Pirner (BP) in [11] transforming the stationary Dirac Hamiltonian to a unitary equivalent even form, came out known to the choice \( \Gamma = \beta \). Based on that perception the perturbative approach initiated in [11] for static external fields, suitable to expand the limiting value of their Hamiltonian flow in powers of \( \frac{c}{v} \), has been generalized in the above as well to apply to a relativistic fermion with minimal coupling to time-dependent electromagnetic fields. Different from [11] though, in view of the initial data of the flow, the electric potential term \( E \) has been considered in order of magnitude being comparable to the kinetic energy term \( \mathcal{O} \) for reasons of consistency with the nonrelativistic limit.

At order \( \frac{v^4}{c^4} \) the relativistic correction to the kinetic energy, the Darwin term and the spin-orbit interaction terms emerge, but taking into account coupling to time-dependent electromagnetic fields now the spin-orbit interaction term manifestly couples to the longitudinal and to the transversal electric field, this result being in full agreement with the result obtained early on by the step-by-step FW-transformation method [2][42].

But at the next order \( \frac{v^6}{c^6} \) the results obtained with the Hamiltonian flow equation approach reveal a discrepancy with results obtained by the (elaborate) step-by-step unitary transformation method of Foldy and Wouthuysen. Comparing these results obtained for the special
case of electrostatic and magnetostatic fields superposed, unfortunately also a discrepancy with the unambiguous energy-separating Eriksen transformation method is manifest.

So, in view of the Hamiltonian flow equation approach beyond order $\frac{1}{c^4}$ not being equivalent to the Eriksen transformation either, a purpose-built reverse beta-flow equation approach was introduced striving for $s \to \infty$ to the energy-sign operator of the stationary Dirac-Hamiltonian. That beta-flow equation being a Riccati equation, serendipitously the exact solution was found and a unitary transformation was constructed in terms of that solution, which turned out to coincide with the Eriksen transformation in the limit $s \to \infty$.

Based on this insight a link between the generators of the Hamiltonian flow and the generator of the reverse beta-flow was noticed, that finally enabled to derive the central results of this article, namely Eq. (126) and Eq. (144), that way fully implementing a convenient energy-separating scheme to unambiguously reconstruct the expansion in powers of $\frac{v}{c}$ for the Newton-Wigner Hamiltonian of the relativistic fermion moving in the presence of electrostatic and magnetostatic fields superposed.

Finally, the results obtained for static fields have been generalized to a Dirac Hamiltonian with coupling to weak amplitude and slowly varying time-dependent electromagnetic fields, resulting in a series expansion of the NW-Hamiltonian in powers of $\frac{v}{c}$ fully coinciding with the correction scheme for the step-by-step FW-transformation method introduced by Silenko [37].

So, the long standing problem of obtaining the explicit series expansion in the parameter $\frac{v}{c}$ of the unitary transformation of a general Dirac Hamiltonian to an even and energy-separating guise, and concurrently being fully in accord with results obtainable with the unambiguous Eriksen transformation, has been resolved.

In view of the step-by-step FW-transformation method not leading to an unambiguous energy-separating result, it would be interesting to apply the introduced flow equation approach as well to bosons carrying mass and charge with spin $S=0$ (Klein-Gordon) or spin $S=1$ (Proca), taking into account coupling to external electromagnetic fields, in this way checking the results obtained early on by Case [4].

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There is a typo in the original article of Foldy and Wouthuysen regarding the sign of the scalar potential term in the Hamiltonian, see their Eq. (34) in [2]. Consequently the sign of the Darwin term in their Eq.(35) is incorrect, whereas the sign of the spin-orbit term is correct. We caution the reader that in the article of Silenko [30], see his Eq.(40), the sign of the spin-orbit term is incorrect, while then again the sign of the scalar potential term and that one of the Darwin term is correct.
Supplemental Material for MS entitled

"A Flow Equation Approach Striving towards an Energy-Separating Hamiltonian Unitary Equivalent to the Dirac Hamiltonian with Coupling to Electromagnetic Fields"

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Abstract

The ensuing comprises supplemental material for the following sections in [1]:

**XIV:** "Perturbation Series for Generator \( \omega(s) \) of Beta-Flow".

**XV:** "Perturbation Series for Operator \( \Omega_u(s) \).

**XVI:** "The Relativistic Corrections to the Schrödinger-Pauli Hamiltonian \( H^{(SP)} \) as a Series Progressing in \( \frac{v^2}{c^2} \).

**SUPPLEMENTAL MATERIAL FOR SECTION XIV IN [1]**

Mind that Eq.(148) in [1] is a nonlinear ODE and therefore more than one solution may exist. To find the (physical) correct solution the property \( Z(s)Z(s) = 1 \) needs to be implemented into the ansatz Eq.(149) in [1], thus leading for

\[
Q(s) = Z(s)\tilde{H}^{(D)}
\]

to the constraint

\[
Q^\dagger(s)Q(s) = \tilde{H}^{(D)}\tilde{H}^{(D)}
\]

Insertion of the perturbation series ansatz

\[
Q(s) = 1_{4\times4} + \sum_{j=1}^{\infty} \kappa^j (Q^{(j)}(s))^\dagger
\]

and comparing coefficients of equal powers \( \kappa^n \) for \( n = 1, 2, 3, \ldots \) on either side of [2] implies

\[
\begin{pmatrix}
1_{4\times4} + \sum_{j=1}^{\infty} \kappa^j (Q^{(j)}(s))^\dagger \\
1_{4\times4} + \sum_{j'=1}^{\infty} \kappa^{j'} Q^{(j')}(s)
\end{pmatrix} = \tilde{H}^{(D)}\tilde{H}^{(D)} = 1_{4\times4} + \sum_{n=2}^{4} \kappa^n R^{(n)}
\]

, or equivalently

\[
\kappa \left( (Q^{(1)}(s))^\dagger + Q^{(1)}(s) \right) + \sum_{n=2}^{\infty} \kappa^n \left( (Q^{(n)}(s))^\dagger + Q^{(n)}(s) \right)
\]

\[
= \sum_{n=2}^{\infty} \kappa^n R^{(n)} - \sum_{j=1}^{\infty} \kappa^j (Q^{(j)}(s))^\dagger \sum_{j'=1}^{\infty} \kappa^{j'} Q^{(j')}(s)
\]

\[
= \sum_{n=2}^{\infty} \kappa^n \left( R^{(n)} - \sum_{j=1}^{n-1} (Q^{(j)}(s))^\dagger Q^{(n-j)}(s) \right)
\]

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, whereby $R^{(n)}$ is stated in Eq.(152) in [1]. So we conclude

$$\left(Q^{(1)}(s)\right)^\dagger = -Q^{(1)}(s)$$

$$n \geq 2$$

$$\left(Q^{(n)}(s)\right)^\dagger + Q^{(n)}(s) = R^{(n)} - \sum_{j=1}^{n-1} \left(Q^{(j)}(s)\right)^\dagger Q^{(n-j)}(s) \quad (5)$$

These relations apply for all terms $Q^{(n)}(s)$ solving the recursion (154) in [1].

For $n = 2$ then

$$\left(Q^{(2)}(s)\right)^\dagger + Q^{(2)}(s) = R^{(2)} - \left(Q^{(1)}(s)\right)^\dagger Q^{(1)}(s)$$

$$= \left(2\beta\tilde{\mathcal{E}} + \tilde{\mathcal{O}}^2\right) + Q^{(1)}(s) Q^{(1)}(s) \quad (6)$$

, and in particular for $s = 0$

$$\left(Q^{(2)}(0)\right)^\dagger + Q^{(2)}(0) = \left(2\beta\tilde{\mathcal{E}} + \tilde{\mathcal{O}}^2\right) + \beta\tilde{\mathcal{O}}^2 \tilde{\mathcal{O}}$$

$$= \left(2\beta\tilde{\mathcal{E}} + \tilde{\mathcal{O}}^2\right) - \tilde{\mathcal{O}}^2$$

$$= 2\beta\tilde{\mathcal{E}} \quad (7)$$

, this indeed being consistent with the posed initial values in Eq.(155) in [1].

Analysis of the recursion Eq.(157) in [1] for $\omega^{(n)}(s) = \left(Q^{(n)}(s)\right)^\dagger - Q^{(n)}(s)$ leads to the following results

$$\omega^{(1)}(s) = -2e^{-4s}\beta\tilde{\mathcal{O}} \quad (8)$$

$$\omega^{(2)}(s) = 0_{4\times4}$$

$$\omega^{(3)}(s) = -4e^{-4s} \left[\tilde{\mathcal{O}}, \tilde{\mathcal{E}}\right] + \left(e^{-4s} \left(-\frac{1}{2} + 4s\right) + \frac{e^{-12s}}{2}\right) \beta\tilde{\mathcal{O}}^3$$

$$\omega^{(4)}(s) = \left(e^{-4s} \left(-\frac{1}{2} + 2s\right) + \frac{e^{-8s}}{2}\right) \beta \left[\tilde{\mathcal{O}}, \left(\tilde{\mathcal{E}}\tilde{\mathcal{O}} + \tilde{\mathcal{O}}\tilde{\mathcal{E}}\right)\right]$$

Inserting the elementary integrals resulting from the evaluation of the recursion Eq.(157) in
one finds after some adjustments with help of the identities

\[ \mathcal{O}^2 \left[ \mathcal{O}, \mathcal{E} \right] + \mathcal{O} \left[ \mathcal{O}, \mathcal{E} \right] \mathcal{O} + \left[ \mathcal{O}, \mathcal{E} \right] \mathcal{O}^2 = \left[ \mathcal{O}^3, \mathcal{E} \right] \] (9)

\[ \mathcal{O}^2 \left[ \mathcal{O}, \mathcal{E} \right] \left[ \mathcal{O}, \mathcal{E} \right] \mathcal{O}^2 = \left[ \mathcal{O}, \left( \mathcal{E} \mathcal{O}^2 + \mathcal{O}^2 \mathcal{E} \right) \right] \]

\[ \left[ \mathcal{O}, \left[ \mathcal{O}, \left[ \mathcal{O}, \mathcal{E} \right] \right] \right] = \mathcal{O}^2 \left[ \mathcal{O}, \mathcal{E} \right] + \left[ \mathcal{O}, \mathcal{E} \right] \mathcal{O}^2 - 2 \mathcal{O} \left[ \mathcal{O}, \mathcal{E} \right] \mathcal{O} = \left[ \mathcal{O}^3, \mathcal{E} \right] - 3 \mathcal{O} \left[ \mathcal{O}, \mathcal{E} \right] \mathcal{O} \]

\[ \mathcal{O} \left[ \mathcal{O}, \mathcal{E} \right] \mathcal{O} = \frac{1}{3} \left[ \mathcal{O}^3, \mathcal{E} \right] - \frac{1}{3} \left[ \mathcal{O}, \left[ \mathcal{O}, \mathcal{E} \right] \right] \]

\[ \mathcal{O}^2 \left[ \mathcal{O}, \mathcal{E} \right] + \left[ \mathcal{O}, \mathcal{E} \right] \mathcal{O}^2 = \frac{2}{3} \left[ \mathcal{O}^3, \mathcal{E} \right] + \frac{1}{3} \left[ \mathcal{O}, \left[ \mathcal{O}, \mathcal{E} \right] \right] \]

the result

\[ \omega^{(5)}(s) = \begin{cases} \quad -4e^{-4s} s^2 \beta \left[ \left[ \mathcal{O}, \mathcal{E} \right], \mathcal{E} \right] \\ + \left( e^{-4s} \left( -\frac{1}{12} + \frac{1}{3} s + \frac{2}{3} s^2 \right) - \frac{1}{12} e^{-8s} + e^{-12s} \left( \frac{1}{6} + \frac{2}{3} s \right) \right) \left[ \mathcal{O}, \left[ \mathcal{O}, \left[ \mathcal{O}, \mathcal{E} \right] \right] \right] \\ + \left( e^{-4s} \left( -\frac{1}{6} - \frac{1}{3} s + \frac{16}{3} s^2 \right) + \frac{1}{3} e^{-8s} + e^{-12s} \left( -\frac{1}{6} + \frac{1}{3} s \right) \right) \left[ \mathcal{O}^3, \mathcal{E} \right] \\ + \left( e^{-4s} \left( \frac{1}{4} - 4s^2 \right) - e^{-12s} \left( \frac{1}{8} + 3s \right) - \frac{1}{8} e^{-20s} \right) \beta \mathcal{O}^5 \end{cases} \] (10)

SUPPLEMENTAL MATERIAL FOR SECTION XV IN [1]

Insertion of the perturbation series

\[ \Omega_u(s) = \sum_{n=0}^{\infty} \kappa^{2n+1} \Omega^{(2n+1)}(s) \] (11)

into Eq.(168 in [1]) leads to

\[ \Omega^{(1)}(s) = \int_0^s ds' \omega^{(1)}(s') = \left( -\frac{1}{2} + \frac{e^{-4s}}{2} \right) \beta \mathcal{O} \] (12)
Now, because

$$[\Omega^{(1)} (s'), \omega^{(1)} (s')] = 0_{4 \times 4}$$  \quad (13)$$

all the commutator term \((\text{ad}_{\Omega_u(s')})^{2n} \circ \omega_u (s')\) in Eq. (168) in [1] are actually not small of order \(O(\kappa^{2n+1})\) but small of order \(O(\kappa^{2n+3})\):

\[
(\text{ad}_{\Omega_u(s')})^2 \circ \omega_u (s') = [\Omega_u (s'), [\Omega_u (s'), \omega_u (s')]]
\]

\[
= \sum_{j'=0}^{\infty} \sum_{j''=0}^{\infty} \sum_{j=0}^{\infty} \kappa^{2j''+1} \Omega^{(2j''+1)} (s'), \left[ \sum_{j'=0}^{\infty} \kappa^{2j'+1} \Omega^{(2j'+1)} (s'), \sum_{j=0}^{\infty} \kappa^{2j+1} \omega^{(2j+1)} (s') \right]
\]

\[
= \sum_{j'=0}^{\infty} \sum_{j''=0}^{\infty} \sum_{j=0}^{\infty} \left[ \Omega^{(2j''+1)} (s'), [\Omega^{(2j'+1)} (s'), \omega^{(2j'+1)} (s')] \right] \kappa^{2j''+1} \kappa^{2j'+1} \kappa^{2j+1}
\]

\[
= \sum_{n=0}^{\infty} \kappa^{2n+3} \sum_{j'=0}^{\infty} \sum_{j''=0}^{\infty} \Theta (n - j' - j'') \left[ \Omega^{(2j''+1)} (s'), [\Omega^{(2j'+1)} (s'), \omega^{(2(n-j'-j'')+1)} (s')] \right]
\]

\[
= \sum_{n=1}^{\infty} \kappa^{2n+3} \sum_{j''=0}^{\infty} \sum_{j'=0}^{\infty} \Theta (n - j' - j'') \left[ \Omega^{(2j''+1)} (s'), [\Omega^{(2j'+1)} (s'), \omega^{(2(n-j'-j'')+1)} (s')] \right]
\]

\[
= O (\kappa^5)
\]

\[
, \text{ and for that same reason}
\]

\[
(\text{ad}_{\Omega_u(s')})^{2n} \circ \omega_u (s') = O (\kappa^{2n+3})
\]

\[
n = 1, 2, 3, \ldots
\]

If we are only interested in an expansion up to and including terms of order \(\kappa^6\) it is adequate to ignore in Eq.(168) in [1] all commutator terms but the first one, leading to

\[
\Omega^{(3)} (s) = \int_0^s ds' \omega^{(3)} (s')
\]

\[
= \left\{ \begin{array}{l}
\left( -\frac{1}{4} + e^{-4s} \left( \frac{1}{4} + s \right) \right) \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right] \\
+ \left( \frac{1}{6} - e^{-4s} \left( \frac{1}{6} + s \right) - e^{-12s} \frac{24}{12} \right) \beta \tilde{\mathcal{O}}^3
\end{array} \right.
\]

The determination of the fifth-order term \(\Omega^{(5)} (s)\) requires to evaluate two double com-
mutator terms:

\[\Omega^{(5)} (s) = \left\{ \begin{array}{c}
\int_0^s ds' \omega^{(5)} (s') \\
-\frac{2}{3} \int_0^s ds' \left[ \left[ \Omega^{(1)} (s'), \Omega^{(3)} (s'), \omega^{(1)} (s') \right] + \left[ \Omega^{(1)} (s'), \Omega^{(3)} (s'), \omega^{(3)} (s') \right] \right]
\end{array} \right. \]  

(17)

Noting

\[
\left[ \beta \bar{\varnothing}^3, \beta \bar{\varnothing} \right] = \beta \bar{\varnothing}^3 \beta \bar{\varnothing} - \beta \bar{\varnothing} \beta \bar{\varnothing}^3 = -\bar{\varnothing}^3 \bar{\varnothing} + \bar{\varnothing} \bar{\varnothing}^3 \equiv 0_{4 \times 4}
\]

then

\[
\int_0^s ds' \left[ \Omega^{(1)} (s'), \Omega^{(3)} (s'), \omega^{(3)} (s') \right] = \int_0^s ds' \left( -\frac{1}{2} e^{-4s'} \right)^2 (-4e^{-4s'}) \left[ \beta \bar{\varnothing}, \left[ \beta \bar{\varnothing}, \bar{\varnothing}, \bar{\varnothing} \right] \right]
\]

and

\[
\int_0^s ds' \left[ \Omega^{(1)} (s'), \Omega^{(3)} (s'), \omega^{(1)} (s') \right] = \int_0^s ds' \left( -\frac{1}{2} e^{-4s'} \right) \left( -\frac{1}{4} e^{-4s'} \left( \frac{1}{4} + s' \right) \right) (-2e^{-4s'}) \left( -\left[ \beta \bar{\varnothing}, \left[ \beta \bar{\varnothing}, \bar{\varnothing}, \bar{\varnothing} \right] \right] \right)
\]

Taking into account the identities (9) the commutator term may be rewritten as

\[
\left[ \beta \bar{\varnothing}, \left[ \beta \bar{\varnothing}, \bar{\varnothing}, \bar{\varnothing} \right] \right] = -\bar{\varnothing}^2 \left[ \bar{\varnothing}, \bar{\varnothing} \right] - \left[ \bar{\varnothing}, \bar{\varnothing} \right] \bar{\varnothing}^2 - 2\bar{\varnothing} \left[ \bar{\varnothing}, \bar{\varnothing} \right] \bar{\varnothing} = -\frac{2}{3} \left[ \bar{\varnothing}^3, \bar{\varnothing} \right] - \frac{1}{3} \left[ \bar{\varnothing}, \left[ \bar{\varnothing}, \bar{\varnothing} \right] \right] - 2 \left( \frac{1}{3} \left[ \bar{\varnothing}^3, \bar{\varnothing} \right] - \frac{1}{3} \left[ \bar{\varnothing}, \left[ \bar{\varnothing}, \bar{\varnothing} \right] \right] \right)
\]

That way

\[
\int_0^s ds' \left[ \left[ \Omega^{(1)} (s'), \Omega^{(3)} (s'), \omega^{(1)} (s') \right] + \left[ \Omega^{(1)} (s'), \Omega^{(3)} (s'), \omega^{(3)} (s') \right] \right]
\]

(21)
\[ \Omega^{(5)}(s) = \left( -\frac{1}{8} + e^{-4s} \left( \frac{1}{8} + \frac{1}{2}s + s^2 \right) \right) \beta \left[ \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right], \tilde{\mathcal{E}} \right] + \left( \frac{25}{3144} - e^{-4s} \left( \frac{1}{48} + \frac{1}{6}s + \frac{1}{6}s^2 \right) + \frac{1}{16}e^{-8s} - e^{-12s} \left( \frac{1}{32} + \frac{1}{18}s \right) \right) \left[ \tilde{\mathcal{O}}, \left[ \tilde{\mathcal{O}}, \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right] \right] \right] \]

\[ + \left( \frac{29}{216} - e^{-4s} \left( \frac{5}{38} + \frac{7}{12}s + \frac{4}{3}s^2 \right) - \frac{1}{16}e^{-8s} + e^{-12s} \left( \frac{5}{72} - \frac{1}{30}s \right) \right) \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right] \]

\[ + \left( -\frac{1}{10} + e^{-4s} \left( \frac{5}{16} + \frac{1}{2}s + s^2 \right) + e^{-12s} \left( \frac{1}{32} + \frac{1}{4}s + \frac{1}{160}e^{-20s} \right) \right) \beta \tilde{\mathcal{O}}^5 \]

\[ -\frac{2}{3} \left( -\frac{5}{192} + e^{-4s} \left( \frac{3}{16} - \frac{1}{8}s \right) - \frac{1}{48}e^{-12s} \right) \left( -\frac{4}{3} \left[ \tilde{\mathcal{O}}^3, \tilde{\mathcal{E}} \right] + \frac{1}{3} \left[ \tilde{\mathcal{O}}, \left[ \tilde{\mathcal{O}}, \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right] \right] \right] \right) \]

The searched for Magnus type series expansion in the limit \( s \to \infty \) thus reads

\[ \Omega_u(\infty) = \kappa \Omega^{(1)}(\infty) + \kappa^3 \Omega^{(3)}(\infty) + \kappa^5 \Omega^{(5)}(\infty) + \ldots \]  

\[ = \kappa \left( -\frac{1}{2} \beta \tilde{\mathcal{O}} \right) + \kappa^3 \left( -\frac{1}{4} \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right] + \frac{1}{6} \beta \tilde{\mathcal{O}}^3 \right) \]

\[ + \kappa^5 \left( -\frac{1}{10} \beta \tilde{\mathcal{O}}^5 + \frac{1}{9} \left[ \tilde{\mathcal{O}}^3, \tilde{\mathcal{E}} \right] + \frac{5}{144} \left[ \tilde{\mathcal{O}}, \left[ \tilde{\mathcal{O}}, \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right] \right] \right] - \frac{1}{5} \beta \left[ \left[ \tilde{\mathcal{O}}, \tilde{\mathcal{E}} \right], \tilde{\mathcal{E}} \right] \right) + O(\kappa^7) \]
Restricting to accuracy $O(\kappa^8)$ then

$$H^{(NW)} = \left\{ \begin{align*}
+ \frac{1}{2} (\text{ad}_{\Omega_u})^2 & \circ (\beta + \kappa^2 \tilde{\mathcal{E}}) + \frac{1}{24} (\text{ad}_{\Omega_u})^4 \circ (\beta + \kappa^2 \tilde{\mathcal{E}}) + \frac{1}{720} (\text{ad}_{\Omega_u})^6 \circ (\beta + \kappa^2 \tilde{\mathcal{E}}) \\
- (\text{ad}_{\Omega_u}) \circ \kappa \tilde{\mathcal{O}} - \frac{1}{6} (\text{ad}_{\Omega_u})^3 \circ \kappa \tilde{\mathcal{O}} - \frac{1}{120} (\text{ad}_{\Omega_u})^5 \circ \kappa \tilde{\mathcal{O}} \\
+ O(\kappa^8)
\end{align*} \right\}$$

\[ (24) \]

$$\equiv \beta + \kappa^2 \tilde{h}^{(2)} + \kappa^4 \tilde{h}^{(4)} + \kappa^6 \tilde{h}^{(6)} + O(\kappa^8)$$

At first sight the indicated accuracy $O(\kappa^8)$ holds indeed with $\Omega_u(\infty)$ being expanded according to (11) up to and including the fifth order term $\Omega^{(5)}$, because upon insertion of (11) there holds

$$\text{ad}_{\Omega_u} \circ \mathcal{F} = \sum_{j=0}^{\infty} \kappa^{2j+1} \text{ad}_{\Omega_u^{(j+1)}} \circ \mathcal{F}$$

\[ (25) \]

Therefore

$$\text{ad}_{\Omega_u} \circ \beta = [\Omega^{(1)}, \beta] = \left[ \left( -\frac{1}{2} \beta \tilde{\mathcal{O}} \right), \beta \right] = \mathcal{O}$$

$$\text{ad}_{\Omega_u} \circ \beta \equiv [\Omega^{(1)}, \text{ad}_{\Omega_u} \circ \beta] = \left[ \left( -\frac{1}{2} \beta \tilde{\mathcal{O}} \right), \mathcal{O} \right] = -\beta \tilde{\mathcal{O}}^2$$

$$\text{ad}_{\Omega_u} \circ \beta = [\Omega^{(1)}, (\text{ad}_{\Omega_u})^2 \circ \beta] = \left[ \left( -\frac{1}{2} \beta \tilde{\mathcal{O}} \right), -\beta \tilde{\mathcal{O}}^2 \right] = -\tilde{\mathcal{O}}^3$$

$$\text{ad}_{\Omega_u} \circ \beta = [\Omega^{(1)}, (\text{ad}_{\Omega_u})^3 \circ \beta] = \left[ \left( -\frac{1}{2} \beta \tilde{\mathcal{O}} \right), -\beta \tilde{\mathcal{O}}^3 \right] = \beta \tilde{\mathcal{O}}^4$$

$$\text{ad}_{\Omega_u} \circ \beta = [\Omega^{(1)}, (\text{ad}_{\Omega_u})^4 \circ \beta] = \left[ \left( -\frac{1}{2} \beta \tilde{\mathcal{O}} \right), \beta \tilde{\mathcal{O}}^4 \right] = \tilde{\mathcal{O}}^5$$

$$\text{ad}_{\Omega_u} \circ \beta = [\Omega^{(1)}, (\text{ad}_{\Omega_u})^5 \circ \beta] = \left[ \left( -\frac{1}{2} \beta \tilde{\mathcal{O}} \right), \tilde{\mathcal{O}}^5 \right] = -\beta \tilde{\mathcal{O}}^6$$
and

\[
\text{ad}_{\Omega(1)} \circ \mathcal{O} = \left[ \Omega(1), \mathcal{O} \right] = \left[ \left( -\frac{1}{2} \beta \mathcal{O} \right), \mathcal{O} \right] = -\beta \mathcal{O}^2 \\
(\text{ad}_{\Omega(1)})^2 \circ \mathcal{O} = \left[ \Omega(1), \text{ad}_{\Omega(1)} \circ \mathcal{O} \right] = \left[ \left( -\frac{1}{2} \beta \mathcal{O} \right), -\beta \mathcal{O}^2 \right] = -\mathcal{O}^3 \\
(\text{ad}_{\Omega(1)})^3 \circ \mathcal{O} = \left[ \Omega(1), (\text{ad}_{\Omega(1)})^2 \circ \mathcal{O} \right] = \left[ \left( -\frac{1}{2} \beta \mathcal{O} \right), -\mathcal{O}^3 \right] = \beta \mathcal{O}^4 \\
(\text{ad}_{\Omega(1)})^4 \circ \mathcal{O} = \left[ \Omega(1), (\text{ad}_{\Omega(1)})^3 \circ \mathcal{O} \right] = \left[ \left( -\frac{1}{2} \beta \mathcal{O} \right), \beta \mathcal{O}^4 \right] = \mathcal{O}^5 \\
(\text{ad}_{\Omega(1)})^5 \circ \mathcal{O} = \left[ \Omega(1), (\text{ad}_{\Omega(1)})^4 \circ \mathcal{O} \right] = \left[ \left( -\frac{1}{2} \beta \mathcal{O} \right), \mathcal{O}^5 \right] = -\beta \mathcal{O}^6
\]

This implies it being adequate to terminate the expansion of \( \text{sinh} \left( \text{ad}_{\Omega_n(\infty)} \right) \) and the expansion of \( \text{cosh} \left( \text{ad}_{\Omega_n(\infty)} \right) \) in Eq.(126) in [1] in the manner implemented, as we are here only interested in the terms up to and including the sixth order \( \kappa^6 \).

Observation: for the commutator terms of order \( \kappa^{2n} \) with \( n \geq 2 \) holds

\[
\frac{1}{2} \text{ad}_{\Omega(1)} \circ \text{ad}_{\Omega(2n-1)} \circ \beta + \frac{1}{2} \text{ad}_{\Omega(2n-1)} \circ \text{ad}_{\Omega(1)} \circ \beta = \text{ad}_{\Omega(2n-1)} \circ \mathcal{O} \tag{26}
\]

Demonstration:

\[
\frac{1}{2} \text{ad}_{\Omega(1)} \circ \text{ad}_{\Omega(2n-1)} \circ \beta + \frac{1}{2} \text{ad}_{\Omega(2n-1)} \circ \text{ad}_{\Omega(1)} \circ \beta \\
= \frac{1}{2} \left[ \Omega(1), \left[ \Omega(2n-1), \beta \right] \right] + \frac{1}{2} \left[ \Omega(2n-1), \left[ \Omega(1), \beta \right] \right] \\
= - \left[ \Omega(1), \beta \Omega(2n-1) \right] - \left[ \Omega(2n-1), \beta \Omega(1) \right] \\
= - \left[ \Omega(1), \beta \right] \Omega(2n-1) - \beta \left[ \Omega(1), \Omega(2n-1) \right] - \left[ \Omega(2n-1), \beta \right] \Omega(1) - \beta \left[ \Omega(2n-1), \Omega(1) \right] \\
= 2\beta \Omega(1) \Omega(2n-1) + 2\beta \Omega(2n-1) \Omega(1) \\
= 2\beta \left( -\frac{1}{2} \beta \mathcal{O} \right) \Omega(2n-1) + 2\beta \Omega(2n-1) \left( -\frac{1}{2} \beta \mathcal{O} \right) \\
= -\mathcal{O} \Omega(2n-1) + \Omega(2n-1) \mathcal{O} \\
= \left[ \Omega(2n-1), \mathcal{O} \right] \\
= \text{ad}_{\Omega(2n-1)} \circ \mathcal{O}
\]

This is a happy coincidence, as it implies to achieve accuracy \( O \left( \kappa^{2n} \right) \) for \( n \geq 2 \) now only the terms \( \Omega(1), \Omega(3), ..., \Omega(2n-3) \) are required, because the commutator terms involving \( \Omega(2n-1) \) cancel!

Trivially

\[
\tilde{h}^{(0)} = \beta \tag{27}
\]
, while the second order term, identical to the nonrelativistic Schrödinger-Pauli Hamiltonian, is readily identified as

\[
\tilde{h}^{(2)} = \tilde{\mathcal{E}} + \frac{1}{2} [\Omega^{(1)}, [\Omega^{(1)}, \beta]] - [\Omega^{(1)}, \tilde{\mathcal{O}}] = \tilde{\mathcal{E}} + \frac{1}{2} \beta \tilde{\mathcal{O}}^2
\]  

(28)

Up next the fourth order term

\[
\tilde{h}^{(4)} = \begin{cases} 
+ \frac{1}{2} [\Omega^{(1)}, [\Omega^{(3)}, \beta]] + \frac{1}{2} [\Omega^{(3)}, [\Omega^{(1)}, \beta]] + \frac{1}{24} [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \beta]]] 
+ \frac{1}{2} [\Omega^{(1)}, [\Omega^{(1)}, \tilde{\mathcal{E}}]] 
- \left[\Omega^{(3)}, \tilde{\mathcal{O}}\right] - \frac{1}{8} \left[\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \tilde{\mathcal{O}}]]\right] 
= - \frac{1}{8} \left[\tilde{\mathcal{O}}, [\tilde{\mathcal{O}}, \tilde{\mathcal{E}}]\right] - \frac{1}{8} \beta \tilde{\mathcal{O}}^4
\end{cases}
\]

(29)

The term \( \tilde{h}^{(4)} \) indeed represents all the leading order relativistic corrections to the Schrödinger-Pauli Hamiltonian in a manifestly gauge invariant manner, namely the spin-orbit interaction together with the Darwin term and also comprising the relativistic correction to the kinetic energy term (with the corresponding corrections to the Zeeman-term included in \( \tilde{\mathcal{O}}^4 \)).

The sixth order term we may write, because of the cancellation of the terms involving \( \Omega^{(5)} \), now in the guise

\[
\tilde{h}^{(6)} = \begin{cases} 
+ \frac{1}{2} [\Omega^{(3)}, [\Omega^{(3)}, \beta]] + \frac{1}{2} [\Omega^{(1)}, [\Omega^{(3)}, \tilde{\mathcal{E}}]] + \frac{1}{2} [\Omega^{(3)}, [\Omega^{(1)}, \tilde{\mathcal{E}}]] 
+ \frac{1}{2} [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \beta]]] + \frac{1}{24} [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \beta]]] 
+ \frac{1}{24} [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \beta]]] + \frac{1}{24} [\Omega^{(1)}, [\Omega^{(3)}, [\Omega^{(1)}, \beta]]] 
+ \frac{1}{24} [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \beta]]] 
+ \frac{1}{720} \left[\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \beta]]]\right] 
- \frac{1}{6} \left[\Omega^{(1)}, [\Omega^{(3)}, \tilde{\mathcal{O}}]\right] - \frac{1}{6} \left[\Omega^{(1)}, [\Omega^{(3)}, [\Omega^{(1)}, \tilde{\mathcal{O}}]]\right] - \frac{1}{6} \left[\Omega^{(3)}, [\Omega^{(1)}, [\Omega^{(1)}, \tilde{\mathcal{O}}]]\right] 
- \frac{1}{120} \left[\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \tilde{\mathcal{O}}]]] \right]
\end{cases}
\]

(30)
Making use of

\[ [\Omega^{(1)}, \beta] = \bar{\Omega} \]

\[
[\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \beta]]]]] = -\beta \bar{\Omega}^6
\]

\[
[\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \bar{\Omega}}]]] = -\beta \bar{\Omega}^6
\]

\[
[\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \beta]]] = -\bar{\Omega}^3
\]

\[
[\Omega^{(1)}, [\Omega^{(1)}, \bar{\Omega}]}] = -\bar{\Omega}^3
\]

\[
[\Omega^{(1)}, [\Omega^{(1)}, \beta]] = -\beta \bar{\Omega}^2
\]

\[
[\Omega^{(1)}, \bar{\Omega}] = -\beta \bar{\Omega}^2
\]

then

\[
\tilde{h}^{(6)} = \begin{cases}
\frac{1}{2} [\Omega^{(3)}, [\Omega^{(3)}, \beta]] + \frac{1}{2} [\Omega^{(1)}, [\Omega^{(3)}, \bar{\epsilon}]} + \frac{1}{2} [\Omega^{(3)}, [\Omega^{(1)}, \bar{\epsilon}]] \\
+ \frac{1}{24} [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \beta]]]] \\
+ \frac{1}{24} [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \beta]]]] \\
+ \frac{5}{720} \beta \bar{\Omega}^6 \\
- \frac{1}{8} [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(3)}, \bar{\Omega}]}]] - \frac{1}{8} [\Omega^{(1)}, [\Omega^{(3)}, (\beta \bar{\Omega}^2)]] - \frac{1}{8} [\Omega^{(3)}, (-\bar{\Omega}^3)]
\end{cases}
\]

Let us evaluate

\[
\Omega^{(3)} = \frac{1}{6} \beta \bar{\Omega}^3 - \frac{1}{4} [\bar{\Omega}, \bar{\epsilon}]
\]

\[
[\Omega^{(3)}, \beta] = -\frac{1}{3} \bar{\Omega}^3 + \frac{1}{2} \beta [\bar{\Omega}, \bar{\epsilon}]
\]
\[
[\Omega^{(1)}, [\Omega^{(3)}, \beta]] = \left[\left(-\frac{1}{2} \beta \partial \right), \left(-\frac{1}{3} \partial^3 + \frac{1}{2} \beta \left[\partial, \bar{\partial} \right]\right)\right] \\
= \frac{1}{3} \beta \partial^4 + \frac{1}{4} \left[\partial, \left[\partial, \bar{\partial} \right]\right]
\]

\[
[\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(3)}, \beta]]] = \left[\left(-\frac{1}{2} \beta \partial \right), \left(\frac{1}{3} \beta \partial^4 + \frac{1}{4} \left[\partial, \left[\partial, \bar{\partial} \right]\right]\right)\right] \\
= \frac{1}{3} \beta \partial^5 - \frac{1}{8} \beta \left[\partial, \left[\partial, \left[\partial, \bar{\partial} \right]\right]\right]
\]

\[
[\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(3)}, \beta]]]] = \left[\left(-\frac{1}{2} \beta \partial \right), \left(\frac{1}{3} \beta \partial^5 - \frac{1}{8} \beta \left[\partial, \left[\partial, \left[\partial, \bar{\partial} \right]\right]\right]\right)\right] \\
= -\frac{1}{3} \beta \partial^6 - \frac{1}{16} \left[\partial, \left[\partial, \left[\partial, \left[\partial, \bar{\partial} \right]\right]\right]\right]
\]

In addition

\[
[\Omega^{(3)}, \partial] = \left[\left(-\frac{1}{4} [\partial, \bar{\partial}] + \frac{1}{6} \beta \partial^4\right), \partial\right] \\
= \frac{1}{4} \left[\partial, \left[\partial, \bar{\partial} \right]\right] + \frac{1}{3} \beta \partial^4
\]

\[
[\Omega^{(1)}, [\Omega^{(3)}], \partial] = \left[\left(-\frac{1}{2} \beta \partial \right), \left(\frac{1}{4} \left[\partial, \left[\partial, \bar{\partial} \right]\right] + \frac{1}{3} \beta \partial^4\right)\right] \\
= -\frac{1}{8} \beta \left[\partial, \left[\partial, \left[\partial, \bar{\partial} \right]\right]\right] + \frac{1}{3} \partial^5
\]

\[
[\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(3)}, \partial]]] = \left[\left(-\frac{1}{2} \beta \partial \right), \left(-\frac{1}{8} \beta \left[\partial, \left[\partial, \bar{\partial} \right]\right] + \frac{1}{3} \partial^5\right)\right] \\
= -\frac{1}{3} \beta \partial^6 - \frac{1}{16} \left[\partial, \left[\partial, \left[\partial, \left[\partial, \bar{\partial} \right]\right]\right]\right]
\]

, in addition

\[
[\Omega^{(3)}, (-\beta \partial^2)] = \left[\left(\frac{1}{6} \beta \partial^3 - \frac{1}{4} \left[\partial, \bar{\partial} \right]\right), (-\beta \partial^2)\right] \\
= \frac{1}{3} \partial^5 - \frac{1}{4} \beta \left(\partial^2 \left[\partial, \bar{\partial} \right] + \left[\partial, \bar{\partial} \right] \partial^2\right)
\]

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\[
[
\Omega^{(1)}, [\Omega^{(3)}, (-\beta \mathcal{O}^2)]
\] = \left[\left(-\frac{1}{2} \beta \mathcal{\bar{O}}\right), \left(\frac{1}{3} \bar{\mathcal{O}}^3 - \frac{1}{4} \beta \left(\mathcal{O}^2 \left[\mathcal{\bar{O}}, \mathcal{E}\right] + \left[\mathcal{\bar{O}}, \mathcal{E}\right] \mathcal{O}^2\right)\right)\right]
= -\frac{1}{3} \beta \bar{\mathcal{O}}^6 - \frac{1}{8} \left[\mathcal{\bar{O}}, \left(\mathcal{O}^2 \left[\mathcal{\bar{O}}, \mathcal{E}\right] + \left[\mathcal{\bar{O}}, \mathcal{E}\right] \mathcal{O}^2\right)\right]
\]

, in addition
\[
[\Omega^{(3)}, (-\mathcal{O}^3)] = \left[\left(\frac{1}{6} \beta \mathcal{\bar{O}}^3 - \frac{1}{4} \left[\mathcal{\bar{O}}, \mathcal{E}\right]\right), (-\mathcal{O}^3)\right]
= -\frac{1}{3} \beta \mathcal{O}^6 - \frac{1}{4} \left[\mathcal{\bar{O}}, \left[\mathcal{\bar{O}}, \mathcal{E}\right]\right]
\]

, in addition
\[
\frac{1}{2} \left[\Omega^{(3)}, [\Omega^{(3)}, \beta]\right] = \frac{1}{2} \left[\Omega^{(3)}, (-2 \beta \Omega^{(3)})\right]
= - \left[\Omega^{(3)}, \beta \Omega^{(3)}\right]
= - \left[\Omega^{(3)}, \beta\right] \Omega^{(3)} - \beta \left[\Omega^{(3)}, \Omega^{(3)}\right]_{\text{evaluated at } 0}
= 2 \beta \Omega^{(3)} \Omega^{(3)}
= 2 \beta \left(\frac{1}{6} \beta \mathcal{\bar{O}}^3 - \frac{1}{4} \left[\mathcal{\bar{O}}, \mathcal{E}\right]\right) \left(\frac{1}{6} \beta \mathcal{\bar{O}}^3 - \frac{1}{4} \left[\mathcal{\bar{O}}, \mathcal{E}\right]\right)
= -\frac{1}{18} \beta \mathcal{O}^6 - \frac{1}{12} \left[\mathcal{\bar{O}}, \left[\mathcal{\bar{O}}, \mathcal{E}\right]\right] + \frac{1}{8} \beta \left(\left[\mathcal{\bar{O}}, \mathcal{E}\right]\right)^2
\]

, in addition
\[
[
\Omega^{(1)}, \mathcal{E}\right] = \left[\left(-\frac{1}{2} \beta \mathcal{\bar{O}}\right), \mathcal{E}\right] = -\frac{1}{2} \beta \left[\mathcal{\bar{O}}, \mathcal{E}\right]
\]
\[
[
\Omega^{(1)}, [\Omega^{(1)}, \mathcal{E}]\right] = \left[\left(-\frac{1}{2} \beta \mathcal{\bar{O}}\right), -\frac{1}{2} \beta \left[\mathcal{\bar{O}}, \mathcal{E}\right]\right]
= -\frac{1}{4} \left[\mathcal{\bar{O}}, \left[\mathcal{\bar{O}}, \mathcal{E}\right]\right]
\]
\[
[
\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \mathcal{E}]\right] = \left[\left(-\frac{1}{2} \beta \mathcal{\bar{O}}\right), \left(-\frac{1}{4} \left[\mathcal{\bar{O}}, \left[\mathcal{\bar{O}}, \mathcal{E}\right]\right]\right)\right]
= \frac{1}{8} \beta \left[\mathcal{\bar{O}}, \left[\mathcal{\bar{O}}, \left[\mathcal{\bar{O}}, \mathcal{E}\right]\right]\right]
\]
\[
[
\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, [\Omega^{(1)}, \mathcal{E}]\right] = \left[\left(-\frac{1}{2} \beta \mathcal{\bar{O}}\right), \frac{1}{8} \beta \left[\mathcal{\bar{O}}, \left[\mathcal{\bar{O}}, \left[\mathcal{\bar{O}}, \mathcal{E}\right]\right]\right]\right]
= \frac{1}{16} \left[\mathcal{\bar{O}}, \left[\mathcal{\bar{O}}, \left[\mathcal{\bar{O}}, \left[\mathcal{\bar{O}}, \mathcal{E}\right]\right]\right]\right]
\]

\[
\left[ \Omega^{(3)}, [\Omega^{(1)}, \tilde{E}] \right] = + \frac{1}{12} [\mathcal{O}^3, [\bar{\mathcal{O}}, \tilde{E}]] - \frac{1}{4} \beta (\left[ [\bar{\mathcal{O}}, \tilde{E}] \right])^2
\]

\[
\left[ \Omega^{(3)}, \tilde{E} \right] = - \frac{1}{4} [[\bar{\mathcal{O}}, \tilde{E}], \tilde{E}] + \frac{1}{6} [\bar{\mathcal{O}}^3, \tilde{E}]
\]

\[
\left[ \Omega^{(1)}, [\Omega^{(3)}, \tilde{E}] \right] = \frac{1}{8} \beta \left( [\bar{\mathcal{O}}, [\bar{\mathcal{O}}, \tilde{E}]] + [[\bar{\mathcal{O}}, \tilde{E}], \bar{\mathcal{O}}] \right) + \frac{1}{12} [\bar{\mathcal{O}}^3, [\bar{\mathcal{O}}, \tilde{E}]]
\]

Insertion of the afore calculated commutator terms into the expression (31) leads to

\[
\tilde{h}^{(6)} = \left\{ \begin{array}{l}
\left( -\frac{1}{18} - \frac{1}{24} \cdot 3 + \frac{1}{8} \left( \frac{1}{3} + \frac{1}{3} + \frac{1}{3} \right) + \frac{5}{720} \right) \beta \bar{\mathcal{O}}^6
= \frac{1}{18} \\
\left( \frac{1}{24} + \frac{1}{8} \cdot 4 - \frac{1}{12} + \frac{1}{24} \right) \left[ \bar{\mathcal{O}}^3, [\bar{\mathcal{O}}, \tilde{E}] \right]
= \frac{1}{12}
\end{array} \right.
\]

\[
+ \left( \frac{1}{24} + \frac{1}{8} - \frac{1}{24} \right) \frac{1}{16} \left[ \bar{\mathcal{O}}, [\bar{\mathcal{O}}, \bar{\mathcal{O}}, [\bar{\mathcal{O}}, \tilde{E}]] \right]
= \frac{1}{128}
\]

\[
+ \frac{1}{8} \cdot 8 \left[ \bar{\mathcal{O}}, \left( \mathcal{O}^2 [\bar{\mathcal{O}}, \tilde{E}] + [\bar{\mathcal{O}}, \tilde{E}] \mathcal{O}^2 \right) \right]
\]

\[
+ \frac{1}{16} \beta \left( \bar{\mathcal{O}} \left[ [\bar{\mathcal{O}}, \tilde{E}], \tilde{E} \right] + [[\bar{\mathcal{O}}, \tilde{E}], \tilde{E}] \bar{\mathcal{O}} \right)
\]

\[
+ \left( \frac{1}{8} - \frac{1}{8} \right) \beta (\left[ [\bar{\mathcal{O}}, \tilde{E}] \right])^2
\]

\[
= 0
\]

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and finally

\[
\tilde{h}^{(6)} = \begin{cases} 
\frac{1}{16} \beta \tilde{O}^6 \\
\frac{1}{32} \left[ \tilde{O}^3, \left[ \tilde{O}, \tilde{\mathcal{E}} \right] \right] \\
+ \frac{1}{128} \left[ \tilde{O}, \left[ \tilde{O}, \left[ \tilde{O}, \left[ \tilde{O}, \tilde{\mathcal{E}} \right] \right] \right] \right] \\
+ \frac{1}{64} \left[ \tilde{O}, \left( \tilde{\mathcal{O}}^2 \left[ \tilde{O}, \tilde{\mathcal{E}} \right] + \left[ \tilde{O}, \tilde{\mathcal{E}} \right] \tilde{\mathcal{O}}^2 \right) \right] \\
+ \frac{1}{16} \beta \left( \tilde{O} \left[ \left[ \tilde{O}, \tilde{\mathcal{E}} \right], \tilde{\mathcal{E}} \right] + \left[ \left[ \tilde{O}, \tilde{\mathcal{E}} \right], \tilde{\mathcal{E}} \right] \tilde{O} \right)
\end{cases}
\]  

(32)

Note that the obtained sixth order term \( \tilde{h}^{(6)} \) in (32) comprises no term being proportional to the square of the electric field. As we have seen, such a term will be represented by \( \beta \left( \left[ \tilde{O}, \tilde{\mathcal{E}} \right] \right)^2 \), but it’s weight cancels to zero. This is in contrast to the expansion found by Brüning et al. [2] and indicates the result of these authors, regarding their higher order terms, being not in accord with the criterion of energy energy-separation, as required for the unitary transformation of the Dirac Hamiltonian to a \( 2 \times 2 \)-blockdiagonal guise being determined unambiguously [3, [4, [1]]].

Last not least, for comparison of our result with results of De Vries and Jonker [5], actually obtained by computer algebra with help of the Pauli-Achieser-Berestezki elimination method [6], let us expand

\[
\left[ \tilde{O}^3, \left[ \tilde{O}, \tilde{\mathcal{E}} \right] \right] = \tilde{O}^4 \tilde{\mathcal{E}} - \tilde{O}^3 \tilde{\mathcal{E}} \tilde{O} - \tilde{O} \tilde{\mathcal{E}} \tilde{O}^3 + \tilde{\mathcal{E}} \tilde{O}^4
\]

\[
\left[ \tilde{O}, \left[ \tilde{O}, \left[ \tilde{O}, \left[ \tilde{O}, \tilde{\mathcal{E}} \right] \right] \right] \right] = \tilde{O}^4 \tilde{\mathcal{E}} - 4 \tilde{O}^3 \tilde{\mathcal{E}} \tilde{O} + 6 \tilde{O}^2 \tilde{\mathcal{E}} \tilde{O}^2 - 4 \tilde{O} \tilde{\mathcal{E}} \tilde{O}^3 + \tilde{\mathcal{E}} \tilde{O}^4
\]

\[
\left[ \tilde{O}, \left( \tilde{\mathcal{O}}^2 \left[ \tilde{O}, \tilde{\mathcal{E}} \right] + \left[ \tilde{O}, \tilde{\mathcal{E}} \right] \tilde{\mathcal{O}}^2 \right) \right] = \tilde{O}^4 \tilde{\mathcal{E}} - 2 \tilde{O}^3 \tilde{\mathcal{E}} \tilde{O} + 2 \tilde{O}^2 \tilde{\mathcal{E}} \tilde{O}^2 - 2 \tilde{O} \tilde{\mathcal{E}} \tilde{O}^3 + \tilde{\mathcal{E}} \tilde{O}^4
\]
Then

\[
\frac{1}{32} \left[ \dot{\mathcal{O}}^3, [\dot{\mathcal{O}}, \ddot{\mathcal{E}}] \right] + \frac{1}{128} \left[ \dot{\mathcal{O}}, [\dot{\mathcal{O}}, [\dot{\mathcal{O}}, \ddot{\mathcal{E}}]] \right] + \frac{1}{64} \left[ \dot{\mathcal{O}}, (\mathcal{O}^2 [\dot{\mathcal{O}}, \ddot{\mathcal{E}}] + [\dot{\mathcal{O}}, \ddot{\mathcal{E}}] \mathcal{O}^2) \right]
\]

\[
= \left\{ \frac{1}{32} \left( \dot{\mathcal{O}}^4 \dddot{\mathcal{E}} - \dot{\mathcal{O}}^3 \dddot{\mathcal{E}} \mathcal{O} - \dot{\mathcal{O}} \dddot{\mathcal{E}} \mathcal{O}^3 + \dddot{\mathcal{E}} \mathcal{O}^4) \right) \right.
\]
\[
+ \frac{1}{128} \left( \dot{\mathcal{O}}^4 \dddot{\mathcal{E}} - 4 \dot{\mathcal{O}}^3 \dddot{\mathcal{E}} \mathcal{O} + 6 \dot{\mathcal{O}}^2 \dddot{\mathcal{E}} \mathcal{O}^2 - 4 \dot{\mathcal{O}} \dddot{\mathcal{E}} \mathcal{O}^3 + \dddot{\mathcal{E}} \mathcal{O}^4 \right)
\]
\[
+ \frac{1}{64} \left( \dot{\mathcal{O}}^4 \dddot{\mathcal{E}} - 2 \dot{\mathcal{O}}^3 \dddot{\mathcal{E}} \mathcal{O} + 2 \dot{\mathcal{O}}^2 \dddot{\mathcal{E}} \mathcal{O}^2 - 2 \dot{\mathcal{O}} \dddot{\mathcal{E}} \mathcal{O}^3 + \dddot{\mathcal{E}} \mathcal{O}^4 \right)
\]
\[
= \left\{ \frac{1}{32} \left[ \dot{\mathcal{O}} \dddot{\mathcal{E}} + \dddot{\mathcal{E}} \mathcal{O}^2 \right] \left( \frac{1}{32} + \frac{1}{128} + \frac{1}{64} \right) \right.
\]
\[
= \left\{ \frac{1}{32} \left[ \dot{\mathcal{O}} \dddot{\mathcal{E}} + \dddot{\mathcal{E}} \mathcal{O}^2 \right] \left( \frac{1}{32} + \frac{4}{128} + \frac{2}{64} \right) \right.
\]
\[
= \left\{ \frac{1}{32} \left[ \dot{\mathcal{O}} \dddot{\mathcal{E}} + \dddot{\mathcal{E}} \mathcal{O}^2 \right] \right. \]
\[
+ \frac{6}{128} + \frac{2}{64} \left( \frac{6}{128} + \frac{2}{64} \right) \left( \dddot{\mathcal{E}} \mathcal{O}^2 \right)
\]
\[
= \frac{7}{128} (\dot{\mathcal{O}}^4 \dddot{\mathcal{E}} + \dddot{\mathcal{E}} \mathcal{O}^4) - \frac{3}{32} (\dot{\mathcal{O}}^3 \dddot{\mathcal{E}} \mathcal{O} + \dddot{\mathcal{E}} \mathcal{O}^3) + \frac{5}{64} \dddot{\mathcal{E}} \mathcal{O}^2
\]

Furthermore

\[
\dot{\mathcal{O}} \left[ [\dot{\mathcal{O}}, \dddot{\mathcal{E}}], \dddot{\mathcal{E}} \right] + \left[ [\dot{\mathcal{O}}, \dddot{\mathcal{E}}], \dddot{\mathcal{E}} \right] \dot{\mathcal{O}}
\]

\[
= \left\{ \dot{\mathcal{O}} \left( \dot{\mathcal{O}} \dddot{\mathcal{E}} - \dddot{\mathcal{E}} \mathcal{O} \right) \dddot{\mathcal{E}} - \dddot{\mathcal{E}} \left( \dot{\mathcal{O}} \dddot{\mathcal{E}} - \dddot{\mathcal{E}} \mathcal{O} \right)
\]
\[
+ \left( \dot{\mathcal{O}} \dddot{\mathcal{E}} - \dddot{\mathcal{E}} \mathcal{O} \right) \dddot{\mathcal{E}} \mathcal{O} - \dddot{\mathcal{E}} \left( \dot{\mathcal{O}} \dddot{\mathcal{E}} - \dddot{\mathcal{E}} \mathcal{O} \right) \dot{\mathcal{O}}
\]
\[
= \left\{ \mathcal{O}^2 \dddot{\mathcal{E}}^2 - 2 \dddot{\mathcal{E}} \dddot{\mathcal{E}} \mathcal{O} + \dddot{\mathcal{E}}^2 \mathcal{O}
\]
\[
+ \dddot{\mathcal{E}} \dddot{\mathcal{E}} \mathcal{O} - 2 \dddot{\mathcal{E}} \dddot{\mathcal{E}} \mathcal{O} + \dddot{\mathcal{E}}^2 \mathcal{O}^2
\]
\[
= \mathcal{O}^2 \dddot{\mathcal{E}}^2 + \dddot{\mathcal{E}}^2 \mathcal{O}^2 - 2 \dddot{\mathcal{E}} \dddot{\mathcal{E}} \mathcal{O} - 2 \dddot{\mathcal{E}} \dddot{\mathcal{E}} \mathcal{O} + 2 \dddot{\mathcal{E}}^2 \mathcal{O}
\]

So our expression for \( \bar{h}^{(6)} \) agrees with the results listed in the table of DeVries and Jonker \( \delta \). It also agrees with the result obtained by Silenko with his correction scheme \[7, 8\]
for the original step-by-step transformation of Foldy and Wouthuysen [9]. Note, that the flow equation based approach leading to Eqs.(126), (144) in [1] is by construction energy-separating and therefore doesn’t need any correction scheme.

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