The Projected Single-Particle Dirac Operator for Coulombic Potentials

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Abstract. A sequence of unitary transformations is applied to the one-electron Dirac operator in an external Coulomb potential such that the resulting operator is of the form $\Lambda_+ A\,\Lambda_+ + \Lambda_- A\,\Lambda_-$ to any given order in the potential strength, where Λ_+ and Λ_- project onto the positive and negative spectral subspaces of the free Dirac operator. To first order, $\Lambda_+ A\,\Lambda_+$ coincides with the Brown-Ravenhall operator. Moreover, there exists a simple relation to the Dirac operator transformed with the help of the Foldy-Wouthuysen technique. By defining the transformation operators as integral operators in Fourier space it is shown that they are well-defined and that the resulting transformed operator is p-form bounded. In the case of a modified Coulomb potential, $V = -\gamma x^{-1+\epsilon}$, $\epsilon > 0$, one can even prove subordinacy of the n-th order term in γ with respect to the $n-1$st order term for all $n > 1$, as well as their p-form boundedness with form bound less than one.

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1 Introduction

Consider a relativistic electron in the Coulomb field V, described by the Dirac operator (in relativistic units, $\hbar = c = 1$)

$$H \;=\; D_0 + V, \qquad D_0 := -i\boldsymbol{\alpha}\,\partial/\partial\mathbf{x} + \beta m, \quad V(x) := -\frac{\gamma}{x} \tag{1.1}$$

where D_0 is the free Dirac operator defined in the Hilbert space $L_2(\mathbb{R}^3)\otimes\mathbb{C}^4$. D_0 is self-adjoint on the Sobolev space $H_1(\mathbb{R}^3)\otimes\mathbb{C}^4$ (with $H_\sigma(\mathbb{R}^3) := \{\varphi \in L_2(\mathbb{R}^3) : \int d\mathbf{p}\,|\hat{\varphi}(\mathbf{p})|^2\,(1+p^2)^\sigma < \infty\}$), and its form domain is $H_{1/2}(\mathbb{R}^3)\otimes\mathbb{C}^4$. The potential strength of V is $\gamma := Ze^2$, Z is the nuclear charge number,

$e^2 = (137.04)^{-1}$ the fine structure constant, $\boldsymbol{\alpha}$ and β the Dirac matrices and $x := |\mathbf{x}|$ [14]. A hat on a function denotes its Fourier transform.
It is well-known that H is not bounded from below. As long as pair creation is neglected, the conventional way to circumvent this deficiency is the introduction of the semibounded operator $P_+ H P_+$ where P_+ projects onto the positive spectral subspace of H. As a first approximation, Brown and Ravenhall [1] introduced the operator

$$B := \Lambda_+ H \Lambda_+, \qquad \Lambda_\pm := \frac{1}{2}\left(1 \pm \frac{D_0}{|D_0|}\right) \tag{1.2}$$

with Λ_+ projecting onto the positive spectral subspace of the free Dirac operator D_0, and $|D_0| = \sqrt{D_0^2}$ is the free energy. In momentum space one has

$$\tilde{D}_0(\mathbf{p}) := \left(\frac{D_0}{|D_0|}\right)(\mathbf{p}) = \frac{\boldsymbol{\alpha}\mathbf{p} + \beta m}{E_p}, \qquad E_p := \sqrt{p^2 + m^2} \tag{1.3}$$

with the electron mass m. By construction, the Brown-Ravenhall operator B is of first order in the potential V and has been shown to be bounded from below for subcritical potential strength γ [5].
An alternative way to derive a semibounded operator from H has been suggested by Douglas and Kroll [4], using the Foldy-Wouthuysen transformation technique [6]. The decoupling of the positive and negative spectral subspaces of H to order n in V is achieved by means of $n+1$ successive unitary transformations U_j', $j = 0, 1, ..., n$

$$(U_n' \cdots U_1' \cdot U_0')\, H\, (U_n' \cdots U_1' \cdot U_0')^{-1} =: H_n' + R_{n+1} \tag{1.4}$$

which cast the tranformed operator into a block-diagonal contribution H_n' plus an error term R_{n+1} with potential strength given by the $n+1$st power of γ. U_0' is the free Foldy-Wouthuysen transformation which block-diagonalises D_0 exactly [14],

$$U_0' := A\left(1 + \beta\,\frac{\boldsymbol{\alpha}\mathbf{p}}{E_p + m}\right), \qquad A := \left(\frac{E_p + m}{2E_p}\right)^{\frac{1}{2}}, \tag{1.5}$$

and for U_j', Douglas and Kroll [4] use

$$U_j' = (1 + W_j^2)^{\frac{1}{2}} + W_j, \qquad j = 1, ..., n \tag{1.6}$$

with antisymmetric operators W_j. It should be noted that the choice of U_j' is not unique, and neither is the resulting operator H_n' from (1.4) for $n > 4$ as has been shown by Wolf, Reiher, and Hess [15]. Applying the free Foldy-Wouthuysen transformation (1.5) one obtains [4, 9]

$$U_0' H U_0'^{-1} = \beta E_p + \mathcal{E}_1 + \mathcal{O}_1$$

$$\mathcal{E}_1 := A\left(V + \frac{\boldsymbol{\alpha}\mathbf{p}}{E_p + m} V \frac{\boldsymbol{\alpha}\mathbf{p}}{E_p + m}\right) A, \quad \mathcal{O}_1 := \beta A \left(\frac{\boldsymbol{\alpha}\mathbf{p}}{E_p + m} V - V \frac{\boldsymbol{\alpha}\mathbf{p}}{E_p + m}\right) A \tag{1.7}$$

where the transformed potential has been split into an even term $\mathcal{E}_1$ (commuting with β) and an odd term $\mathcal{O}_1$ (anticommuting with β, since $\alpha_k \beta = -\beta\alpha_k, \;\; k = 1, 2, 3$). For an exponential unitary transformation,

$$U_j' := e^{-iS_j}, \qquad\qquad j = 1, ..., n \tag{1.8}$$

with a symmetric operator S_j, the next transformation gives in agreement with [9]

$$e^{-iS_1} U_0' H U_0'^{-1} e^{iS_1} = \beta E_p + \mathcal{E}_1 + \mathcal{O}_1 + i[\beta E_p, S_1] + i[\mathcal{E}_1 + \mathcal{O}_1, S_1]$$
$$-\frac{1}{2}\,[\,[\beta E_p, S_1],\, S_1] + R_3. \tag{1.9}$$

S_1 is defined from the requirement that $\mathcal{O}_1$ is eliminated,

$$i\,[\beta E_p, S_j] = -\mathcal{O}_j, \qquad\qquad j = 1 \tag{1.10}$$

hence S_1 is odd and of first order in the potential like $\mathcal{O}_1$. After each transformation U_j', the $j + 1$st order term in γ of R_{j+1} is decomposed into even ($\mathcal{E}_{j+1}$) and odd ($\mathcal{O}_{j+1}$) contributions, and the successive transformation $U_{j+1}' = e^{-iS_{j+1}}$ is chosen to eliminate $\mathcal{O}_{j+1}$, which is achieved by the condition (1.10) for the $j > 1$ under consideration. With this procedure one arrives at the even (and hence block-diagonal) operator

$$H_n' = \beta E_p + \mathcal{E}_1 + ... + \mathcal{E}_n. \tag{1.11}$$

The physical quantity of interest is the expectation value of the transformed Dirac operator. For the Brown-Ravenhall operator, consider the expectation value formed with 4-spinors φ in the positive spectral subspace of D_0 which in momentum space can be expressed in terms of Pauli spinors $u \in H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^2$,

$$\hat{\varphi}(\mathbf{p}) = \frac{1}{\sqrt{2E_p\,(E_p + m)}} \begin{pmatrix} (E_p + m)\;\hat{u}(\mathbf{p}) \\ \mathbf{p}\boldsymbol{\sigma}\;\hat{u}(\mathbf{p}) \end{pmatrix} \tag{1.12}$$

where $\boldsymbol{\sigma}$ is the vector of the three Pauli matrices. Then, an operator b_m acting on $H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^2$ may be defined by [5]

$$(\varphi, B\varphi) =: (u, b_m u). \tag{1.13}$$

On the other hand, in case of the Douglas-Kroll transformed operator H_n', its upper block corresponds to the particle states (having positive energy) and therefore the expectation value has to be formed with the four-spinor $\psi := \binom{u}{0}$ with $u \in H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^2$ as above.

For the first-order term, H_1', it is easy to show [2] that its expectation value agrees with the expectation value of the Brown-Ravenhall operator, i.e.

$$(u, b_m u) \;=\; \left(\binom{u}{0}, H_1' \binom{u}{0} \right), \qquad\qquad u \in H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^2, \tag{1.14}$$

such that H_n' may be considered as the natural continuation of B to higher order in V. While H_n' is known explicitly up to $n = 5$ [15], the spectral properties, in particular the boundedness from below, have only been investigated for the Jansen-Hess operator (i.e. $n = 2$) [2, 8].
The aim of this work is to prove two theorems.

Theorem 1.1. *Let $H = D_0 + V$ be the one-particle Dirac operator acting on $\mathcal{S}(\mathbb{R}^3) \otimes \mathbb{C}^4$ with $\mathcal{S}$ the Schwartz space of smooth strongly localised functions. Let γ be the strength of the Coulomb potential V and $p := |\mathbf{p}|$. Then there exists a sequence of unitary transformations $U_k = e^{iB_k}$, $k = 1, ..., n$, such that the transformed Dirac operator can be written in the following way*

$$(U_1 \cdots U_n)^{-1} H \, U_1 \cdots U_n \;=:\; H^{(n)} \;+\; R^{(n+1)}$$

$$H^{(n)} \;:=\; \Lambda_+ \left(\sum_{k=0}^{n} H_k \right) \Lambda_+ \;+\; \Lambda_- \left(\sum_{k=0}^{n} H_k \right) \Lambda_-. \tag{1.15}$$

Here, Λ_+ projects onto the positive spectral subspace of D_0, $\Lambda_- = 1 - \Lambda_+$, and H_k is a p-form bounded operator, its form bound being proportional to γ^k, $k = 1, ..., n$. The remainder $R^{(n+1)}$ which still couples the spectral subspaces of D_0 is p-form bounded with form bound $O(\gamma^{n+1})$ when γ tends to zero. The operators B_k are symmetric and bounded, extending to self-adjoint operators on $L_2(\mathbb{R}^3) \otimes \mathbb{C}^4$.

An operator H_k with the properties stated in the theorem is said to be *of order* γ^k.
It is shown below that $H_0 := D_0$ and $H_1 := V$ such that to first order, the Brown-Ravenhall operator B is recovered. (1.15) implies that the transformed Dirac operator can be expressed in terms of projectors to arbitrary order in the potential strength. Similar transformation schemes are known for bounded operators on lattices, see e.g. [3] and [13].
The next theorem states the unitary equivalence of the transformed Dirac operators obtained with either the transformation scheme from Theorem 1.1 or the Douglas-Kroll transformation scheme (1.8) - (1.11).

Theorem 1.2. *Let $\varphi \in \Lambda_+(\mathcal{S}(\mathbb{R}^3) \otimes \mathbb{C}^4)$ be a 4-spinor in the positive spectral subspace of D_0, which defines a Pauli spinor u by means of (1.12). Let H_n' be the Douglas-Kroll transformed Dirac operator to n-th order in the potential strength, obtained with exponential unitary operators U_j'. Then to any order n, its expectation value agrees with the one of the transformed Dirac operator* *from (1.15),*

$$(\varphi, H^{(n)}\,\varphi) \;=\; \left(\varphi, \sum_{k=0}^{n} H_k\,\varphi\right) \;=\; \left(\begin{pmatrix}u\\0\end{pmatrix}, H_n' \begin{pmatrix}u\\0\end{pmatrix}\right), \qquad n=1,2,\ldots\,. \tag{1.16}$$

This extends the first-order equation (1.14) to arbitrary order n. Actually (1.16) holds also for other types of unitary operators, provided the same type is used in all transformations U_k and U_k', $k \geq 1$.

2 Proof of Theorem 1.1

2.1 Derivation of unitary transformations

The sequence of unitary operators $U_k = e^{iB_k}$ is constructed with the help of an iteration scheme. Following Sobolev [13] we consider U_k as an element of the group $U_k(t) = e^{iB_k t}$, $t \in \mathbb{R}$.
Let A be an arbitrary t-independent operator. The derivative of the transformed operator is given by

$$\frac{d}{dt}A(t) := \frac{d}{dt}\left(e^{-iB_k t}\,A\,e^{iB_k t}\right) \;=\; i\,U_k(-t)\;[A,B_k]\;U_k(t) \tag{2.1}$$

where the commutator $[A,B_k] := AB_k - B_kA$. This equation is easily integrated, noting that $A(0)=A$,

$$A(t) \;=\; U_k(-t)\,A\,U_k(t) \;=\; A \;+\; i\int_0^t d\tau\;U_k(-\tau)\;[A,B_k]\;U_k(\tau). \tag{2.2}$$

Iterating once, i.e. replacing A by the operator $[A,B_k]$ in (2.2) and inserting the resulting equation into the r.h.s. of (2.2), one obtains for $t=1$

$$A(1) \;=\; A \,+\, i[A,B_k] \,+\, i^2\int_0^1 d\tau \int_0^\tau dt'\,U_k(-t')\,[[A,B_k],B_k]\,U_k(t'). \tag{2.3}$$

After n iterations the following representation of A_1 is obtained,

$$A(1) \,=\, A + i[A,B_k] \,+\, \frac{1}{2!}i^2\;[[A,B_k],B_k] \;+ \ldots +\; \frac{1}{n!}i^n\;[[\ldots[A,B_k],\ldots,B_k] \;+\; R \tag{2.4}$$

where the n-th term contains n commutators with B_k, and the remainder R is an $(n+1)$-fold integral.
Let us apply this scheme inductively to the Dirac operator $H = D_0 + V$. Assume that to order $n-1$ the transformation has been achieved with a resulting operator of the form given in Theorem 1.1,

$$(U_1\cdots U_{n-1})^{-1}\;H\;U_1\cdots U_{n-1} \;=\; H^{(n-1)} \;+\; H_n \;+\; \tilde{R}^{(n+1)} \tag{2.5}$$

where H_n and $\tilde{R}^{(n+1)}$ are respectively of order γ^n and γ^{n+1}, and still couple the spectral subspaces. Decompose H_n into

$$H_n \;=\; V_n \;+\; W_n, \qquad\qquad V_n := \;\Lambda_+ H_n \Lambda_+ \;+\; \Lambda_- H_n \Lambda_-$$
$$W_n := \;\Lambda_+ H_n \Lambda_- \;+\; \Lambda_- H_n \Lambda_+ \,. \tag{2.6}$$

The next transformation, $U_n = e^{iB_n}$, aims at eliminating the term W_n which, in contrast to V_n, couples the spectral subspaces. This condition will fix B_n. We note that from (2.4), the transformation reproduces the operator itself, such that the term $H^{(n-1)}$, already in the desired form, is preserved. From this it follows that $H^{(n-1)}$ contains the zero-order term $\Lambda_+ D_0 \Lambda_+ + \Lambda_- D_0 \Lambda_- \; = D_0$ (note that $\Lambda_\pm$ commutes with D_0 and $\Lambda_+^2 + \Lambda_-^2 = 1$).
We obtain

$$U_n^{-1}\,(H^{(n-1)} \,+\, H_n)\,U_n \;=\; H^{(n-1)} \,+\, V_n \,+\, W_n \,+\, i[D_0, B_n] \tag{2.7}$$
$$+\, i\,[(\Lambda_+ \sum_{k=1}^{n-1} H_k \Lambda_+ \,+\, \Lambda_- \sum_{k=1}^{n-1} H_k \Lambda_-),\, B_n] \;+\; \tilde{R},$$

where $\tilde{R}$ collects the terms containing at least two commutators with B_n. B_n is determined from the requirement

$$W_n \;+\; i\,[D_0, B_n] \;=\; 0. \tag{2.8}$$

Since W_n is of order γ^n, B_n is proportional to γ^n (the boundedness of B_n is shown later). Moreover, the commutators of the type $[(\Lambda_+ H_k \Lambda_+ + \Lambda_- H_k \Lambda_-), B_n]$ are of order γ^{n+k} with $k \geq 1$, and $\tilde{R}$ is of order γ^{2n}. Hence, these terms are disregarded (together with the remainder $\tilde{R}^{(n+1)}$ from (2.5)) in constructing the transformed operator to order n,

$$H^{(n)} \;=\; H^{(n-1)} \;+\; V_n \;=\; D_0 \,+\, V_1 \,+\, V_2 + ... + V_n. \tag{2.9}$$

Particularly interesting are the cases $n = 1$ and $n = 2$. For $n = 1$, we have

$$H^{(1)} \;=\; D_0 \;+\; V_1 \;=\; \Lambda_+\,(D_0 + V)\,\Lambda_+ \;+\; \Lambda_-\,(D_0 + V)\,\Lambda_-. \tag{2.10}$$

Restricting $H^{(1)}$ to the positive spectral subspace $\Lambda_+(\mathcal{S}(\mathbb{R}^3) \otimes \mathbb{C}^4)$, the second term on the r.h.s. of (2.10) vanishes and the remaining term agrees with the Brown-Ravenhall operator.
Let us now consider $n = 2$. From (2.9) it follows that the transformed Dirac operator in second order is determined by the first transformation, $U_1 = e^{iB_1}$, only. However, the existence of the second transformation, $U_2 = e^{iB_2}$, has to be established to show that $H^{(2)}$ is indeed the transformed operator, with a remainder of order γ^3. We have

$$U_1^{-1}\,H\,U_1 \;=\; D_0 + V_1 + W_1 \,+\, i\,[D_0, B_1] \,+\, i\,[V, B_1] \,-\, \frac{1}{2}[[D_0, B_1], B_1] \,+\, R,$$

$$R \;=\; -\int_0^1 d\tau \int_0^\tau dt'\; U_1(-t')\; [[V,B_1],B_1]\; U_1(t') \tag{2.11}$$

$$-\,i\int_0^1 d\tau \int_0^\tau dt' \int_0^{t'} d\tau'\; U_1(-\tau')\; [[[D_0,B_1],B_1],B_1]\; U_1(\tau').$$

Making use of the defining relation for B_1, $W_1 + i[D_0,B_1] = 0$, the operator $H^{(2)}$ takes the form

$$H^{(2)} \;=\; D_0 + V_1 \;+\; \Lambda_+ H_2 \Lambda_+ \;+\; \Lambda_- H_2 \Lambda_- \tag{2.12}$$

$$H_2 := \; i\,[V_1,B_1] \;+\; \frac{i}{2}[W_1,B_1].$$

2.2 Integral operators in Fourier space and the determination of B_1

Since D_0 is a multiplication operator in momentum space, it is convenient to set up the calculus in Fourier space. Let $\varphi \in \mathcal{S}(\mathbb{R}^3)\otimes\mathbb{C}^4$. We define an integral operator W acting on φ by means of

$$(W\,\varphi)(\mathbf{x}) := \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p}\; e^{i\mathbf{p}\mathbf{x}}\, w(\mathbf{x},\mathbf{p})\; \hat\varphi(\mathbf{p}) \tag{2.13}$$

where here and in the following the (three-dimensional) momentum integrals extend over the whole $\mathbb{R}^3$. This agrees with the formal definition of a pseudodifferential operator [13] and we will call $w(\mathbf{x},\mathbf{p})$ the symbol of W. Introducing the Fourier transform $\hat w(\mathbf{q},\mathbf{p})$, $W\varphi$ takes the form

$$(W\,\varphi)(\mathbf{x}) \;=\; \frac{1}{(2\pi)^3} \int d\mathbf{p}\; e^{i\mathbf{p}\mathbf{x}} \int d\mathbf{q}\; e^{i\mathbf{q}\mathbf{x}}\; \hat w(\mathbf{q},\mathbf{p})\; \hat\varphi(\mathbf{p}). \tag{2.14}$$

From this, the Fourier transform of $W\varphi$ is found

$$(\widehat{W\varphi})(\mathbf{p}') \;=\; \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p}\; \hat w(\mathbf{p}'-\mathbf{p},\mathbf{p})\; \hat\varphi(\mathbf{p}). \tag{2.15}$$

With φ in (2.14) replaced by $G\varphi$, the symbol of a product WG of two integral operators is derived,

$$(W\,G\,\varphi)(\mathbf{x}) \;=\; \frac{1}{(2\pi)^3} \int d\mathbf{p}'\; e^{i\mathbf{p}'\mathbf{x}} \int d\mathbf{p}\; \hat w(\mathbf{p}'-\mathbf{p},\mathbf{p})\; \widehat{G\varphi}(\mathbf{p}). \tag{2.16}$$

Using (2.15) for $\widehat{G\varphi}(\mathbf{p})$, as well as the definition (2.14) of the Fourier transformed symbol $\widehat{wg}$ of WG, one gets

$$\widehat{wg}(\mathbf{q},\mathbf{p}) \;=\; \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p}'\; \hat w(\mathbf{q}-\mathbf{p}',\mathbf{p}+\mathbf{p}')\; \hat g(\mathbf{p}',\mathbf{p}). \tag{2.17}$$

For the goal of determining the transformation U_1, its exponent B_1 is considered as an integral operator. One has to solve (2.8) for $n = 1$, using $W_1 = \Lambda_+ V \Lambda_- + \Lambda_- V \Lambda_+$ and (1.2),

$$-i\,[D_0, B_1] \;=\; W_1 \;=\; \frac{1}{2}\left(V \;-\; \frac{D_0}{|D_0|}\,V\,\frac{D_0}{|D_0|}\right). \tag{2.18}$$

Let ϕ_1 be the symbol of B_1. From (2.14) and with D_0 from (1.1) one has

$$(D_0\,B_1\,\varphi)(\mathbf{x}) \;=\; \frac{1}{(2\pi)^3}\int d\mathbf{p}\,d\mathbf{q}\,D_0\,e^{i(\mathbf{p}+\mathbf{q})\mathbf{x}}\;\hat{\phi}_1(\mathbf{q},\mathbf{p})\;\hat{\varphi}(\mathbf{p})$$

$$=\;\frac{1}{(2\pi)^3}\int d\mathbf{p}\,d\mathbf{q}\,[\boldsymbol{\alpha}(\mathbf{p}+\mathbf{q}) \;+\; \beta m]\;e^{i(\mathbf{p}+\mathbf{q})\mathbf{x}}\;\hat{\phi}_1(\mathbf{q},\mathbf{p})\;\hat{\varphi}(\mathbf{p}). \tag{2.19}$$

The Fourier transforms of $D_0\varphi$ and of $V\varphi$ are, respectively, obtained from

$$(\widehat{D_0\varphi})(\mathbf{p}) \;=\; (\boldsymbol{\alpha}\mathbf{p} \;+\; \beta m)\;\hat{\varphi}(\mathbf{p})$$

$$(V\,\varphi)(\mathbf{x}) \;=\; \frac{1}{(2\pi)^{3/2}}\int d\mathbf{q}\;e^{i\mathbf{q}\mathbf{x}}\left(-\frac{\gamma}{2\pi^2 q^2}\right)\int d\mathbf{p}\;e^{i\mathbf{p}\mathbf{x}}\;\hat{\varphi}(\mathbf{p}) \tag{2.20}$$

such that the symbol v of V is defined by $\hat{v}(\mathbf{q},\mathbf{p}) \;=\; -\sqrt{2/\pi}\,\gamma/q^2$. Acting (2.18) on φ and equating the respective symbols leads to the following algebraic equation for $\hat{\phi}_1$:

$$[\boldsymbol{\alpha}(\mathbf{p}+\mathbf{q}) \;+\; \beta m]\;\hat{\phi}_1(\mathbf{q},\mathbf{p}) \;-\; \hat{\phi}_1(\mathbf{q},\mathbf{p})\;[\boldsymbol{\alpha}\mathbf{p} + \beta m] \;=\; i\;\hat{w}_1(\mathbf{q},\mathbf{p}) \tag{2.21}$$

$$=\;-\frac{i\gamma_0}{q^2}\;[1 \;-\; \tilde{D}_0(\mathbf{q}+\mathbf{p})\cdot\tilde{D}_0(\mathbf{p})]$$

with $\gamma_0 \;:=\; \gamma/\sqrt{2\pi}$ and $\tilde{D}_0(\mathbf{p})$ the operator from (1.3) with norm unity. $\hat{w}_1(\mathbf{q},\mathbf{p})$, behaving like q^{-1} for $q \to 0$, is less singular than $\hat{v}(\mathbf{q},\mathbf{p})$, such that the prescription (2.6) for W_1 implies a regularisation of the potential V.

Lemma 2.1. *A solution $\hat{\phi}_1(\mathbf{q},\mathbf{p})$ for the symbol of B_1 is given by*

$$\hat{\phi}_1(\mathbf{q},\mathbf{p}) \;=\; -\frac{i\gamma_0}{q^2}\;\frac{1}{E_p + E_{|\mathbf{q}+\mathbf{p}|}}\;\left(\tilde{D}_0(\mathbf{q}+\mathbf{p}) \;-\; \tilde{D}_0(\mathbf{p})\right) \tag{2.22}$$

which satisfies the condition for symmetry of B_1 [13],

$$\hat{\phi}_1(-\mathbf{q},\mathbf{p}+\mathbf{q})^* \;=\; \hat{\phi}_1(\mathbf{q},\mathbf{p}). \tag{2.23}$$

It is estimated by

$$|\hat{\phi}_1(\mathbf{q},\mathbf{p})| \;\le\; \frac{c}{q}\;\frac{1}{(q+p+1)^2} \tag{2.24}$$

with some constant $c \in \mathbb{R}_+$. B_1 is a bounded operator on $L_2(\mathbb{R}^3)\otimes\mathbb{C}^4$.

Proof. a) Calculation of $\hat{\phi}_1$.

In order to solve (2.21) the ansatz is made

$$\hat{\phi}_1(\mathbf{q},\mathbf{p}) \;=\; -\frac{i\gamma_0}{q^2}\,(c_1\boldsymbol{\alpha}\mathbf{q} \;+\; c_2\boldsymbol{\alpha}\mathbf{p} \;+\; c_3\beta) \tag{2.25}$$

and from the properties of the Dirac matrices $\beta^2 = 1,\ \alpha_i^2 = 1,\ \beta\alpha_i = -\alpha_i\beta,\ i = 1,2,3,\ \ \alpha_i\alpha_k = -\alpha_k\alpha_i\ (i \neq k)$, the following identities are derived

$$\boldsymbol{\alpha}\mathbf{p}\cdot\boldsymbol{\alpha}\mathbf{p} \;=\; p^2, \qquad\qquad \boldsymbol{\alpha}\mathbf{q}\cdot\boldsymbol{\alpha}\mathbf{p} \;=\; 2\mathbf{pq} \;-\; \boldsymbol{\alpha}\mathbf{p}\cdot\boldsymbol{\alpha}\mathbf{q}. \tag{2.26}$$

Insertion of (2.25) into (2.21) then leads to an equation of the type

$$\lambda_1\,\boldsymbol{\alpha}\mathbf{p}\cdot\boldsymbol{\alpha}\mathbf{q} \;+\; \lambda_2\,\boldsymbol{\alpha}\mathbf{q}\cdot\beta \;+\; \lambda_3\,\boldsymbol{\alpha}\mathbf{p}\cdot\beta \;+\; \lambda_4 \;=\; 0 \tag{2.27}$$

where the $\lambda_k,\ \ k = 1,...,4,$ are scalars depending on $\mathbf{p}$ and $\mathbf{q}$. (2.27) must hold for $\mathbf{p},\mathbf{q} \in \mathbb{R}^3$ whence $\lambda_k = 0,\ \ k = 1,...,4$. The resulting system of 4 equations for the $c_i,\ \ i = 1,2,3$ has a unique solution,

$$c_1\,(q^2{+}2\mathbf{pq}) \;=\; 1 - \frac{E_p}{E_{|\mathbf{q}+\mathbf{p}|}}, \qquad c_2 \;=\; 2c_1 - \frac{1}{E_p\,E_{|\mathbf{q}+\mathbf{p}|}}, \qquad c_3 \;=\; c_2 m \tag{2.28}$$

such that

$$\hat{\phi}_1(\mathbf{q},\mathbf{p}) = -\frac{i\gamma_0}{q^2}\left[[(\mathbf{q}{+}2\mathbf{p})\boldsymbol{\alpha}{+}2\beta m]\frac{1}{q^2{+}2\mathbf{pq}}\left(1 - \frac{E_p}{E_{|\mathbf{q}+\mathbf{p}|}}\right) - \frac{\mathbf{p}\boldsymbol{\alpha}+\beta m}{E_pE_{|\mathbf{q}+\mathbf{p}|}}\right]. \tag{2.29}$$

It is readily verified that (2.29) can be cast into the form (2.22), proving that $\hat{\phi}_1(\mathbf{q},\mathbf{p})$ is continuous in both variables except for $q = 0$.

b) The symmetry condition (2.23) follows immediately from (2.22) using the self-adjointness of $\boldsymbol{\alpha}$ and β.

c) We define the class of our integral operators (2.14) by means of the estimate of their symbols in the six-dimensional space $(\mathbf{q},\mathbf{p}) \in \mathbb{R}^6$. This estimate determines the convergence properties of integrals without the precise knowledge of the symbols themselves, and it is an easy way to deal with products of integral operators in proofs of boundedness or p-form boundedness.

In order to estimate a symbol by its asymptotic behaviour for $q,p \to 0$ and $q,p \to \infty$, it must be a continuous function of the two variables in $\mathbb{R}_+ \times \mathbb{R}_+$. This condition is fulfilled for $\hat{\phi}_1(\mathbf{q},\mathbf{p})$. By inspection of (2.22) one finds that $\hat{\phi}_1(\mathbf{q},\mathbf{p})$ is finite $\neq 0$ for $p = 0$ while it behaves $\sim 1/q,\ \ q \to 0,\ \ \sim 1/q^3,\ \ q \to \infty$ and $\sim 1/p^2,\ \ p \to \infty$. Taken into consideration that $\phi_1(\mathbf{x},\mathbf{p})$ is dimensionless as is B_1 (cf. $U_1 = e^{iB_1}$ and (2.13)) whence $\hat{\phi}_1(\mathbf{q},\mathbf{p})$ is of dimension $(\text{momentum})^{-3}$, the estimate

$|\hat{\phi}_1(\mathbf{q},\mathbf{p})| \leq c/q\cdot(q+p+1)^{-2}$ is obtained. The constant c is determined by the maximum of $q\cdot|\hat{\phi}_1(\mathbf{q},\mathbf{p})|$ in $q,p\in\mathbb{R}_+$ (which exists due to continuity) and by the decay constants of $\hat{\phi}_1(\mathbf{q},\mathbf{p})$ for $q\to\infty$ and $p\to\infty$, respectively (maximised in the second variable).

d) We present here only the proof of the form boundedness of B_1; the operator boundedness can be shown along the same lines.

The basic ingredient is the *Lieb and Yau formula* which is a consequence of the Schur test [12] and which also can be derived from Schwarz's inequality [11]. We give it in a slightly generalised form,

$$\left|\int d\mathbf{q}\,d\mathbf{p}\;\overline{\hat{\varphi}(\mathbf{q})}\;|K(\mathbf{q},\mathbf{p})\,|\;\hat{\varphi}(\mathbf{p})\right| \tag{2.30}$$

$$\leq\left(\int d\mathbf{q}d\mathbf{p}|\hat{\varphi}(\mathbf{p})|^2|K(\mathbf{q},\mathbf{p})|\left|\frac{f(p)}{f(q)}\right|^2\right)^{\frac{1}{2}}\cdot\left(\int d\mathbf{q}d\mathbf{p}|\hat{\varphi}(\mathbf{p})|^2|K(\mathbf{p},\mathbf{q})|\left|\frac{f(p)}{f(q)}\right|^2\right)^{\frac{1}{2}}$$

with $f(p)>0$ for $p>0$ a smooth convergence generating function. For a symmetric kernel, $K(\mathbf{p},\mathbf{q}) = K(\mathbf{q},\mathbf{p})$, (2.30) simplifies to the conventional form [11, 5].

From the condition (2.23) we have the following symmetry with respect to interchange of $\mathbf{q}$ and $\mathbf{p}$,

$$|\hat{\phi}_1^*(\mathbf{q}-\mathbf{p},\mathbf{p})| \;=\; |\hat{\phi}_1(\mathbf{p}-\mathbf{q},\mathbf{q})| \;\overset{\mathbf{q}\leftrightarrow\mathbf{p}}{\mapsto}\; |\hat{\phi}_1(\mathbf{q}-\mathbf{p},\mathbf{p})|. \tag{2.31}$$

One then obtains for $\varphi\in L_2(\mathbb{R}^3)\otimes\mathbb{C}^4$ applying (2.15) and subsequently (2.30) and (2.31)

$$|(\varphi,B_1\varphi)| = |(\hat{\varphi},\widehat{B_1\varphi})| \;\leq\; \frac{1}{(2\pi)^{\frac{3}{2}}}\int d\mathbf{q}\,|\overline{\hat{\varphi}(\mathbf{q})}|\int d\mathbf{p}\,|\hat{\phi}_1(\mathbf{q}-\mathbf{p},\mathbf{p})|\,|\hat{\varphi}(\mathbf{p})| \tag{2.32}$$

$$\leq \frac{1}{(2\pi)^{\frac{3}{2}}}\left(\int d\mathbf{q}\,d\mathbf{p}\,|\hat{\varphi}(\mathbf{p})|^2\,|\hat{\phi}_1(\mathbf{q}-\mathbf{p},\mathbf{p})|\left|\frac{f(p)}{f(q)}\right|^2\right)^{\frac{1}{2}}$$

$$\cdot\left(\int d\mathbf{q}\,d\mathbf{p}\,|\hat{\varphi}(\mathbf{p})|^2\,|\hat{\phi}_1^*(\mathbf{q}-\mathbf{p},\mathbf{p})|\left|\frac{f(p)}{f(q)}\right|^2\right)^{\frac{1}{2}}.$$

Both symbol and its adjoint can be estimated by the same expression (2.24) (from (2.22) one even has $\hat{\phi}_1^*(\mathbf{q},\mathbf{p}) = -\hat{\phi}_1(\mathbf{q},\mathbf{p})$), yielding

$$|(\varphi,B_1\varphi)| \;\leq\; \frac{c}{(2\pi)^{\frac{3}{2}}}\int d\mathbf{p}\;|\hat{\varphi}(\mathbf{p})|^2\;\cdot I_1(p)$$

$$I_1(p) := \int d\mathbf{q}\;\frac{1}{|\mathbf{q}-\mathbf{p}|}\;\frac{1}{(|\mathbf{q}-\mathbf{p}|\;+p+1)^2}\;\left|\frac{f(p)}{f(q)}\right|^2. \tag{2.33}$$

For the form boundedness of B_1 it remains to prove that $I_1(p)$ is bounded for $p \in \mathbb{R}_+$. The angular integration is performed with the help of the formula

$$\int_{-1}^{1} dx \, \frac{1}{\sqrt{b+ax}} \, \frac{1}{(\sqrt{b+ax}\,+p+1)^2} \;=\; \frac{2}{a} \int_{\sqrt{b-a}}^{\sqrt{b+a}} \frac{dz}{(z+p+1)^2}$$

$$= \; \frac{2}{a} \left(\frac{1}{\sqrt{b-a}\,+p+1} \;-\; \frac{1}{\sqrt{b+a}\,+p+1} \right) \tag{2.34}$$

identifying $|\mathbf{q}-\mathbf{p}| \;=\; \sqrt{q^2+p^2-2qpx} \;=:\; \sqrt{b+ax}, \quad x \;:=\; \cos\vartheta_{\mathbf{q},\mathbf{p}}$. Choosing $f(p) := p^{\frac{1}{2}}$, one obtains

$$I_1(p) = 2\pi \int_0^\infty dq \left(\frac{1}{|q-p|+p+1} - \frac{1}{q+2p+1} \right) = 4\pi \ln \frac{2p+1}{p+1} < \infty. \tag{2.35}$$

□

As a consequence of the boundedness on $L_2(\mathbb{R}^3) \otimes \mathbb{C}^4$ and the symmetry, B_1 is self-adjoint and $U_1 = e^{iB_1}$ is unitary.

2.3 Existence of B_2 and the transformations of higher order

Let ϕ_n denote the symbol of B_n. It is briefly indicated how ϕ_2 can be obtained explicitly, but for B_n, $\;n \geq 2$, the calculus with operator classes is applied instead. B_2 is defined by

$$-i[D_0,B_2] = W_2 = i\Lambda_+ \Big[[V_1,B_1] + \frac{1}{2}[W_1,B_1] \Big] \Lambda_- + i\Lambda_- \Big[[V_1,B_1] + \frac{1}{2}[W_1,B_1] \Big] \Lambda_+. \tag{2.36}$$

With W_1 from (2.18) and $V_1 = V - W_1$ one obtains

$$W_2 \;=\; \frac{i}{8} \, \Big(3\,[V,B_1] \;+\; [\tilde{D}_0, V\tilde{D}_0\,B_1] \;+\; [\tilde{D}_0, B_1\tilde{D}_0 V] \;+\; 3\,\tilde{D}_0\,[B_1,V]\,\tilde{D}_0 \Big). \tag{2.37}$$

(2.36) is, like the corresponding equation for B_1, solved in momentum space by introducing the respective symbols of the operators. The Fourier transformed symbol $\hat{w}_2$ of W_2 is composed of expressions of the type (cf (2.17))

$$\widehat{v\phi_1}(\mathbf{q},\mathbf{p}) \;=\; -\frac{\gamma}{2\pi^2} \int d\mathbf{p}' \, \frac{1}{|\mathbf{q}-\mathbf{p}'|^2} \, \hat{\phi}_1(\mathbf{p}',\mathbf{p}) \tag{2.38}$$

where $\widehat{v\phi_1}$ is the Fourier transformed symbol of the product VB_1. This implies that — in contrast to (2.21) — the equation for $\hat{\phi}_2(\mathbf{p},\mathbf{q})$,

$$[\boldsymbol{\alpha}\,(\mathbf{p}+\mathbf{q}) \;+\; \beta m]\;\hat{\phi}_2(\mathbf{q},\mathbf{p}) \;-\; \hat{\phi}_2(\mathbf{q},\mathbf{p})\;[\boldsymbol{\alpha}\mathbf{p} \;+\beta m] \;=\; i\,\hat{w}_2(\mathbf{q},\mathbf{p}), \tag{2.39}$$

involves an extra integral on the r.h.s. and is solved with the ansatz (using (2.22) for $\hat{\phi}_1(\mathbf{p}',\mathbf{p})$)

$$\hat{\phi}_2(\mathbf{q},\mathbf{p}) \;=\; -\frac{i\gamma\gamma_0}{16\pi^2}\int d\mathbf{p}'\,\frac{1}{p'^2}\,\frac{1}{|\mathbf{q}-\mathbf{p}'|^2}\;(c_1 \;+\; c_2\,\boldsymbol{\alpha}\mathbf{p}\cdot\beta m$$

$$+\,c_3\,\boldsymbol{\alpha}\mathbf{q}\cdot\beta m \;+\; c_4\,\boldsymbol{\alpha}\mathbf{p}'\cdot\beta m \;+\; c_5\,\boldsymbol{\alpha}\mathbf{p}'\cdot\boldsymbol{\alpha}\mathbf{p} \;+\; c_6\,\boldsymbol{\alpha}\mathbf{q}\cdot\boldsymbol{\alpha}\mathbf{p} \;+\; c_7\,\boldsymbol{\alpha}\mathbf{q}\cdot\boldsymbol{\alpha}\mathbf{p}')\,. \tag{2.40}$$

The scalar coefficients $c_j,\;\; j=1,...,7$ (depending on $\mathbf{q},\mathbf{p}$ and $\mathbf{p}'$) are uniquely determined.

The matter of interest is, however, not the explicit form of B_2 or generally, of $B_n,\;\; n\geq 2,$ but the existence of the potentials W_n and V_n on the form domain $H_{1/2}(\mathbb{R}^3)\otimes\mathbb{C}^4$ of the free Dirac operator, such that the expectation value of $H^{(n)}$ from (2.9) is well defined.

Lemma 2.2. *Let $U_n = e^{iB_n},\;\; n\geq 1,$ be the transformations from Theorem 1.1. Let ϕ_n be the symbol of B_n and W_n the potential in the defining equation for ϕ_n. Then W_n is p-form bounded on $H_{1/2}(\mathbb{R}^3)\otimes\mathbb{C}^4$ by means of*

$$|(\varphi, W_n\varphi)| \;\leq\; c\,(\varphi, p\,\varphi) \tag{2.41}$$

with $c\in\mathbb{R}_+$, and B_n extends to a bounded operator on $L_2(\mathbb{R}^3)\otimes\mathbb{C}^4$.

From the inductive definition of the transformation scheme it is easily seen that W_n is symmetric. As a consequence of (2.8), B_n is symmetric and hence self-adjoint, such that U_n is unitary for all $n\geq 1$.

Proof.

a) p-form boundedness of W_n

The proof is by induction. The p-form boundedness of W_1, eq. (2.18), follows from Kato's inequality [10] and from the self-adjointness and boundedness of $\tilde{D}_0$,

$$|(\varphi, W_1\varphi)| \;\leq\; \frac{1}{2}\,|(\varphi, V\varphi)| \;+\; \frac{1}{2}\,|(\tilde{D}_0\varphi, V\tilde{D}_0\varphi)| \;\leq\; \frac{\gamma\pi}{4}\,(\varphi,p\varphi) \;+\; \frac{\gamma\pi}{4}\,(\varphi,p\varphi) \tag{2.42}$$

where in the second term, $\tilde{D}_0 p \tilde{D}_0 = p$ has been used.

Let $n\geq 2$. According to the transformation scheme outlined in section 2.1, W_n is composed of multiple commutators of V with $B_k,\;\; k<n.$ In particular for $n=2,\;\; [V,B_1]$ contributes (see (2.37)) and for $n=3$, one needs $[[V,B_1],B_1]$ and $[V,B_2]$. The additionally occurring factors $\tilde{D}_0$ can be disregarded in the context of p-form boundedness since $\tilde{D}_0$ is a bounded multiplication operator in momentum space. In the general case, the product of all factors $B_k,\;\; k\leq n-1,$ which enter into a given commutator contributing to W_n must be proportional to γ^{n-1} since W_n is of the order γ^n.

By induction hypothesis, W_k is p-form bounded on $H_{1/2}(\mathbb{R}^3)\otimes\mathbb{C}^4$ for $k\leq n-1$. This means that all commutators of smaller order than n in γ are

p-form bounded. In the induction step one has to show that $[V, B_{n-1}]$ and $[[\cdot], B_k]$, $k < n-1$, are p-form bounded where $[\cdot]$ denotes a p-form bounded multiple commutator.

Without loss of generality one may assume that $[\cdot]$ is symmetric. This guarantees the symmetry property (2.31) for the Fourier transformed symbol $\widehat{[\cdot]}(\mathbf{p},\mathbf{q})$. We estimate $|\widehat{[\cdot]}| \leq |\widehat{[\cdot]}| + |\widehat{[\cdot]}^*|$ and apply the Lieb and Yau formula for this symmetrised kernel. Then, using that a symbol can be estimated by its adjoint and vice versa, p-form boundedness can be expressed in the following way

$$|(\varphi,[\cdot]\varphi)| \leq \frac{1}{(2\pi)^{\frac{3}{2}}} \int d\mathbf{p}\, |\hat{\varphi}(\mathbf{p})|^2 \int d\mathbf{q} \left(\left|\widehat{[\cdot]}(\mathbf{q}-\mathbf{p},\mathbf{p})\right| + \left|\widehat{[\cdot]}^*(\mathbf{q}-\mathbf{p},\mathbf{p})\right| \right) \left|\frac{f(p)}{f(q)}\right|^2$$

$$\leq \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p}\ |\hat{\varphi}(\mathbf{p})|^2\ c\,p \ =\ c'\ (\varphi, p\,\varphi) \tag{2.43}$$

with some constant $c > 0$. The inequality in the second line of (2.43) restricts the convergence generating function to $f(p) := p^\lambda$ with $\frac{1}{2} < \lambda < \frac{3}{2}$. This is true because both $\widehat{[\cdot]}(\mathbf{q}-\mathbf{p},\mathbf{p})$ and $\widehat{[\cdot]}(\mathbf{p}-\mathbf{q},\mathbf{q})$ are regular for $q \to 0$ (since all operators of which $[\cdot]$ is composed have symbols which are regular when the second variable tends to zero), restricting $\lambda < \frac{3}{2}$, and because $\widehat{[\cdot]}$ is of dimension (momentum)$^{-2}$, decreasing like q^{-2} for $q \to \infty$, such that $\lambda > \frac{1}{2}$ is required. These properties hold also for the symmetric operator W_k. Thus for $k < n$ when W_k is p-form bounded, (2.43) therefore is also valid for its Fourier transformed symbol $\hat{w}_k$ in place of $\widehat{[\cdot]}$.

Another ingredient in the proof of p-form boundedness of W_n is the fact that the symbol ϕ_n can be estimated by w_n. First note that the estimate of $\hat{\phi}_n$ is related to the estimate of $\hat{w}_n$ by an equation of the type (2.39), derived from the defining equation (2.8). This equation implies that the behaviour of $\hat{\phi}_n$ for $p \to 0$ and $q \to 0$ is that of $\hat{w}_n$, while there occurs an extra power of q^{-1} and p^{-1} for $q \to \infty$ and $p \to \infty$, respectively. Therefore

$$|\hat{\phi}_n(\mathbf{q},\mathbf{p})| \ \leq\ \frac{c}{q+p+1}\,|\hat{w}_n(\mathbf{q},\mathbf{p})|. \tag{2.44}$$

i) p-form boundedness of $[V, B_{n-1}]$

From the symmetry of V, B_{n-1} and (2.15) we get

$$|(\varphi,[V,B_{n-1}]\varphi)| \ \leq\ |(\widehat{V\varphi},\widehat{B_{n-1}\varphi})| \ +\ |(\widehat{B_{n-1}\varphi},\widehat{V\varphi})|$$

$$\leq \frac{1}{(2\pi)^3} \int d\mathbf{p}' d\mathbf{p}\, d\mathbf{q}\, |\hat{\varphi}(\mathbf{p})| \Big\{ |\hat{v}^*(\mathbf{p}'-\mathbf{p},\mathbf{p})|\, |\hat{\phi}_{n-1}(\mathbf{p}'-\mathbf{q},\mathbf{q})|$$

$$+\ |\hat{\phi}^*_{n-1}(\mathbf{p}'-\mathbf{p},\mathbf{p})|\, |\hat{v}(\mathbf{p}'-\mathbf{q},\mathbf{q})| \Big\}\, |\hat{\varphi}(\mathbf{q})|. \tag{2.45}$$

Due to the symmetry in $\mathbf{p}$ and $\mathbf{q}$, the Lieb and Yau formula can be applied in the same way as in (2.32) and in (2.43). Using $f(p) := p$ for the convergence generating function and estimating $\hat{v}$ one gets

$$|(\varphi,[V,B_{n-1}]\,\varphi)| \;\le\; c\int d\mathbf{p}\;|\hat{\varphi}(\mathbf{p})|^2\;\left\{\int d\mathbf{p}'\;\frac{1}{|\mathbf{p}'-\mathbf{p}|^2}\,\frac{p^2}{p'^2}\cdot\int d\mathbf{q}\right.$$

$$\left.\left|\hat{\phi}_{n-1}(\mathbf{p}'-\mathbf{q},\mathbf{q})\right|\frac{p'^2}{q^2}\;+\!\int\! d\mathbf{p}'\left|\hat{\phi}_{n-1}(\mathbf{p}-\mathbf{p}',\mathbf{p}')\right|\frac{p^2}{p'^2}\cdot\!\int\! d\mathbf{q}\frac{1}{|\mathbf{p}'-\mathbf{q}|^2}\frac{p'^2}{q^2}\right\}. \tag{2.46}$$

The last $\mathbf{q}$-integral is evaluated with the substitution $\mathbf{q}' := \mathbf{q}/p'$ and with $\mathbf{e}_{p'} := \mathbf{p}'/p'$,

$$\int\! d\mathbf{q}\frac{1}{|\mathbf{q}-\mathbf{p}'|^2}\frac{p'^2}{q^2} = p'\!\int_0^\infty\! dq'\!\int_{S^2}\! d\Omega_{q'}\frac{1}{|\mathbf{q}'-\mathbf{e}_{p'}|^2} = 2\pi p'\!\int_0^\infty\frac{dq'}{q'}\ln\left|\frac{1+q'}{1-q'}\right|$$
$$= \pi^3 p'. \tag{2.47}$$

Also $\hat{\phi}_{n-1}$ is estimated by $\hat{w}_{n-1}$ via (2.44). One obtains for the second term in curly brackets of (2.46) with the help of the p-form boundedness of W_{n-1} by means of (2.43)

$$\int\! d\mathbf{p}'|\hat{\phi}_{n-1}(\mathbf{p}-\mathbf{p}',\mathbf{p}')|\frac{p^2}{p'^2}\cdot\pi^3 p' \le \tilde{c}\!\int\! d\mathbf{p}'\frac{1}{|\mathbf{p}-\mathbf{p}'|+p'+1}\,|\hat{w}_{n-1}(\mathbf{p}-\mathbf{p}',\mathbf{p}')|\frac{p^2}{p'}$$
$$\le c''p \tag{2.48}$$

where $|\mathbf{p}-\mathbf{p}'|+p'+1\;\ge p'$ has been used. Further we note that the factor $(|\mathbf{p}'-\mathbf{q}|+q+1)^{-1}$ is bounded for all $q\ge 0$ and hence can be estimated by its value at $q=0$. We thus get for the other $\mathbf{q}$-integral

$$\int d\mathbf{q}\;|\hat{\phi}_{n-1}(\mathbf{p}'-\mathbf{q},\mathbf{q})|\;\frac{p'^2}{q^2}\;\le\;\frac{\tilde{c}}{p'+1}\;\int d\mathbf{q}\;|\hat{w}_{n-1}(\mathbf{p}'-\mathbf{q},\mathbf{q})|\;\frac{p'^2}{q^2}$$
$$\le\;\frac{\tilde{c}}{p'+1}\cdot cp'\;\le\;\tilde{c}c \tag{2.49}$$

such that by means of (2.47), the first term in the curly brackets of (2.46) is estimated by $c'p$ with some constant $c'\in\mathbb{R}_+$. This proves the p-form boundedness of $[V,B_{n-1}]$.

ii) p-form boundedness of $[[\cdot],B_k]$

In (2.45), V and B_{n-1} are replaced with $[\cdot]$ and B_k, respectively, and the expression in curly brackets (integrated over $\mathbf{p}'$) is taken as the kernel $K(\mathbf{q},\mathbf{p})$ in the Lieb and Yau formula (2.30). Then, estimating the symbol by its adjoint and vice versa, one arrives at

$$|(\varphi,[\,[\cdot],B_k]\,\varphi)|\;\le\;\frac{\tilde{c}}{(2\pi)^3}\int d\mathbf{p}\;|\hat{\varphi}(\mathbf{p})|^2\;\cdot\left\{\int d\mathbf{p}'\;\left|\widehat{[\cdot]}(\mathbf{p}-\mathbf{p}',\mathbf{p}')\right|\;\frac{p^2}{p'^2}\right.$$

$$\cdot \int d\mathbf{q} \left|\hat{\phi}_k(\mathbf{p}'-\mathbf{q},\mathbf{q})\right| \frac{p'^2}{q^2} + \int d\mathbf{p}' \left|\hat{\phi}_k(\mathbf{p}-\mathbf{p}',\mathbf{p}')\right| \frac{p^2}{p'^2} \int d\mathbf{q} \left|\widehat{[\cdot]}(\mathbf{p}'-\mathbf{q},\mathbf{q})\right| \frac{p'^2}{q^2} \Bigg\}. \tag{2.50}$$

By (2.43), the last $\mathbf{q}$-integral is bounded by cp' such that the second term in the curly brackets can be estimated by

$$\int d\mathbf{p}' |\hat{\phi}_k(\mathbf{p}-\mathbf{p}',\mathbf{p}')| \frac{p^2}{p'} \leq c \int d\mathbf{p}' \frac{1}{|\mathbf{p}-\mathbf{p}'|+p'+1} |\hat{w}_k(\mathbf{p}-\mathbf{p}',\mathbf{p}')| \frac{p^2}{p'} \leq c'p \tag{2.51}$$

according to (2.48) because $\hat{w}_k$ is p-form bounded. By (2.49), the other $\mathbf{q}$-integral is estimated by a constant $\tilde{c}$, such that the first term of (2.50) in curly brackets is with (2.43) estimated by $p \cdot c''$ with some constant c''. This proves the p-form boundedness of $[[\cdot], B_k]$, $k < n-1$, and hence together with (i) the p-form boundedness of W_n.

From the p-form boundedness of W_n, $n \geq 1$, on $H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^4$, proven above, follows immediately the p-form boundedness of V_n, $n \geq 1$ since both operators differ only by factors $\tilde{D}_0$. We have therefore proven that to arbitrary order n,

$$|(\varphi, (V_1 + ... + V_n)\,\varphi)| \;\leq\; c\,(\varphi, p\,\varphi) \tag{2.52}$$

for $\varphi \in H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^4$.

b) Boundedness of B_n

This is a consequence of the p-form boundedness of W_n. From (2.43) with $[\cdot]$ replaced by B_n one gets

$$|(\varphi, B_n \varphi)| \;\leq\; \frac{c}{(2\pi)^{3/2}} \int d\mathbf{p}\, |\hat{\varphi}(\mathbf{p})|^2 \int d\mathbf{q}\, |\hat{\phi}_n^*(\mathbf{q}-\mathbf{p},\mathbf{p})|\, \frac{p^2}{q^2} \tag{2.53}$$

where the convergence generating function is again chosen as $f(p) := p$. From (2.49) the $\mathbf{q}$-integral is estimated by a constant. Hence,

$$|(\varphi, B_n \varphi)| \;\leq\; \text{const}\,(\varphi, \varphi). \tag{2.54}$$

□

Remark. Due to logarithmic divergencies occurring in the estimates of $\hat{w}_n(\mathbf{q},\mathbf{p})$, $n \geq 1$, the proof of boundedness of B_n cannot be based on the algebra of symbol estimates, a powerful method in the case of periodic potentials [13].

2.4 The Remainder $R^{(n+1)}$ and its p-form boundedness

From its definition as remainder after multiple iterations of (2.3)-type equations (see e.g. (2.11)), $R^{(n+1)}$ is composed of a finite number of compact integrals over a unitary transform of the same multiple commutators $[\cdot]$ which would contribute to the $n+1$st order term V_{n+1} after one additional transformation (for the commutator involving D_0, use (2.8)). These commutators are p-form bounded according to the proof of Lemma 2.2, and it remains to show that the unitary transform preserves the p-form boundedness. Consider

$$|(\varphi,\, U_k(-\tau)\,[\cdot]\,U_k(\tau)\,\varphi)| \;=\; |(U_k(\tau)\,\varphi,\, [\cdot]\,U_k(\tau)\,\varphi)|$$

$$\leq\; c\,(U_k(\tau)\,\varphi,\, p\,U_k(\tau)\,\varphi) \;=\; c\,(\varphi,\, U_k(-\tau)\,p\,U_k(\tau)\,\varphi). \tag{2.55}$$

Since $U_k(\tau) = e^{iB_k\tau}$ with B_k a bounded operator, we can Taylor expand

$$(\varphi, e^{-iB_k\tau}\,p\,e^{iB_k\tau}\,\varphi) \;\leq\; \sum_{n,m=0}^{\infty} \frac{\tau^n}{n!}\,\frac{\tau^m}{m!}\,|(\varphi, B_k^n\,p\,B_k^m\,\varphi)|. \tag{2.56}$$

The sum on the r.h.s. represents a symmetric operator such that its kernel has the required symmetry property to apply the Lieb and Yau formula (with convergence generating function $f(p) = p$). Our proof proceeds in 4 steps: We prove p-form boundedness of (i) pB_k, (ii) pB_k^m (by induction), (iii) $B_kpB_k^m$, (iv) $B_k^npB_k^m$.

According to (2.32) we establish boundedness of an operator A by means of boundedness of the integral I_A over its Fourier transformed symbol $\hat{s}_A$. For B_k, we have boundedness from (2.49),

$$I_{B_k} := \frac{1}{(2\pi)^{3/2}} \int d\mathbf{q}\,|\hat{\phi}_k(\mathbf{p}-\mathbf{q},\mathbf{q})|\,\frac{p^2}{q^2} \;\leq\; c_k. \tag{2.57}$$

p-form boundedness is proven by showing that the integrals I_A (with $A := B_k^npB_k^m$) are proportional to p.

(i)

$$I_{pB_k} \;=\; \frac{1}{(2\pi)^{3/2}} \int d\mathbf{q}\,p\,|\hat{\phi}_k(\mathbf{p}-\mathbf{q},\mathbf{q})|\,\frac{p^2}{q^2} \;\leq\; p\,c_k. \tag{2.58}$$

(ii) Our induction hypothesis is $I_{pB_k^m} \leq pc_k^m$. We decompose $pB_k^{m+1} = pB_k^m \cdot B_k$ and use (2.17) for the symbol of a product of operators. Then with (2.57),

$$I_{pB_k^{m+1}} \;=\; \frac{1}{(2\pi)^{3/2}} \int d\mathbf{q}'\,|\hat{s}_{pB_k^{m+1}}(\mathbf{p}-\mathbf{q}',\mathbf{q}')|\,\frac{p^2}{q'^2} \tag{2.59}$$

$$\leq \frac{1}{(2\pi)^3} \int d\mathbf{q}\,|\hat{s}_{pB_k^m}(\mathbf{p}-\mathbf{q},\mathbf{q})|\,\frac{p^2}{q^2} \cdot \int d\mathbf{q}'\,|\hat{\phi}_k(\mathbf{q}-\mathbf{q}',\mathbf{q}')|\,\frac{q^2}{q'^2} \leq p\,c_k^m \cdot c_k = p\,c_k^{m+1}.$$

(iii) Decomposing $B_kpB_k^m = B_k \cdot pB_k^m$, one has from (2.51)

$$I_{B_kpB_k^m} \;\leq\; \frac{1}{(2\pi)^3} \int d\mathbf{q}\,|\hat{\phi}_k(\mathbf{p}-\mathbf{q},\mathbf{q})|\,\frac{p^2}{q^2} \cdot \int d\mathbf{q}'\,|\hat{s}_{pB_k^m}(\mathbf{q}-\mathbf{q}',\mathbf{q}')|\,\frac{q^2}{q'^2}$$

$$\leq\; c_k^m\,\frac{1}{(2\pi)^{3/2}} \int d\mathbf{q}\,|\hat{\phi}_k(\mathbf{p}-\mathbf{q},\mathbf{q})|\,\frac{p^2}{q} \;\leq\; c_k^m\,c_k'\,p. \tag{2.60}$$

(iv) We claim $I_{B_k^n p B_k^m} \le p\, c_k^{'n}\, c_k^m$. Then, using (2.60)

$$I_{B_k^{n+1} p B_k^m} \;\le\; \frac{1}{(2\pi)^3} \int d\mathbf{q}\; |\hat{\phi}_k(\mathbf{p}-\mathbf{q},\mathbf{q})|\; \frac{p^2}{q^2} \cdot \int d\mathbf{q}'\; |\hat{s}_{B_k^n p B_k^m}(\mathbf{q}-\mathbf{q}',\mathbf{q}')|\; \frac{q^2}{q'^2}$$

$$\le\; c_k^{'n}\, c_k^m \cdot c_k'\, p \;=\; p\, c_k^{'n+1}\, c_k^m. \tag{2.61}$$

Thus we obtain from the Lieb and Yau formula applied to (2.56)

$$\sum_{n,m=0}^{\infty} \frac{\tau^n}{n!}\,\frac{\tau^m}{m!}\, |(\varphi, B_k^n\, p\, B_k^m\, \varphi)| \;\le\; c \sum_{n,m=0}^{\infty} \frac{\tau^n}{n!}\,\frac{\tau^m}{m!}\, c_k^{'n}\, c_k^m\; (\varphi, p\,\varphi)$$

$$=\; c\, e^{c_k'\tau + c_k\tau}\; (\varphi, p\,\varphi) \tag{2.62}$$

with c a constant resulting from using the same estimate for symbol and its adjoint. This shows that $(\varphi, U_k(-\tau) p U_k(\tau)\varphi)$ is p-form bounded and completes the proof since $\exp(c_k'\tau + c_k\tau)$ is a continuous function of τ. With the same reasoning, any multiple finite-dimensional compact integral over multiple unitary transforms of p-form bounded commutators is therefore again p-form bounded.

3 Subordinacy of the higher-order contributions

Since to any order n the p-form bound of $H^{(n)}$ is proportional to γ^n while for the remainder $R^{(n+1)}$ it is proportional to γ^{n+1}, one gets convergence of the expansion in the strength of the Coulomb field for $\gamma \to 0$. However, for larger $\gamma < 1$, the p-form bounds of V_n obtained with the above estimates can in general not be restricted to numbers less than 1. In this section we will consider a slight modification of the Coulomb potential,

$$V(x) := -\frac{\gamma}{x^{1-\epsilon}}, \qquad \hat{v}(\mathbf{q}) \;=\; -\gamma\sqrt{\frac{2}{\pi}}\;\frac{f_\epsilon}{q^{2+\epsilon}}, \quad \epsilon > 0 \tag{3.1}$$

where $\hat{v}(\mathbf{q})$ is the Fourier transform and $f_\epsilon := \cos\frac{\pi\epsilon}{2} \cdot \Gamma(1+\epsilon) \;\to 1$ for $\epsilon \to 0$. All quantities defined previously will now pertain to the modified potential (3.1).

Our results are collected in the following proposition.

Proposition 3.1. *For the modified Coulomb potential (3.1) we have*

(i) For every $k \in \mathbb{N}$, $\epsilon < \frac{1}{k+1}$, the k-th order potential term V_k is p-form bounded with form bound less than 1.

(ii) Let $\varphi \in \mathcal{S}(\mathbb{R}^3) \otimes \mathbb{C}^4$. Let $\mu_k > 0$ for $k \in \mathbb{N}$ be the infimum of the constant c in the estimate $|(\varphi, V_k\varphi)| \le c\,(\varphi, p^{1-k\epsilon}\varphi)$. Then V_{k+1} is subordinate to V_k in the sense

$$|(\varphi, V_{k+1}\,\varphi)| \;\le\; \delta\, |(\varphi, V_k\varphi)| \;+\; C\,(\varphi,\varphi) \tag{3.2}$$

with $0 < \delta < 1$ and $C \in \mathbb{R}_+$ a constant depending on δ.

(iii) Let $R^{(n+1)} := U_n^* \cdots U_1^* H U_1 \cdots U_n - H^{(n)}$ *be the remainder of order* $n+1$ *in the potential strength. Then* $R^{(n+1)}$ *is subordinate to* V_n*.*

For the proof, a lemma is needed.

Lemma 3.2. *For* $0 < (n+1)\epsilon < 1$, $c_0 \in \mathbb{R}_+$, $n \in \mathbb{N}$ *and every* $\varphi \in H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^4$ *one has*

$$c_0\,(\varphi, p^{1-(n+1)\epsilon}\varphi) \le c\,(\varphi, p^{1-n\epsilon}\varphi) + C\,(\varphi,\varphi) \tag{3.3}$$

with $c < 1$ *and* $C \in \mathbb{R}_+$*. For* $n = 0$ *this implies* p*-form boundedness with form bound* < 1*,*

$$c_0\,(\varphi, p^{1-\epsilon}\varphi) \le c\,(\varphi, p\,\varphi) + C\,(\varphi,\varphi). \tag{3.4}$$

Proof. We use an elementary inequality from analysis,

$$a \cdot b \le \frac{a^\lambda}{\lambda} + \frac{b^\mu}{\mu}, \qquad a, b > 0, \quad \frac{1}{\lambda} + \frac{1}{\mu} = 1, \tag{3.5}$$

choose $\lambda := \frac{1-n\epsilon}{1-(n+1)\epsilon} > 1$, $\mu = \frac{1-n\epsilon}{\epsilon}$ and $0 < \delta < 1$ to be specified later. We decompose

$$p^{1-(n+1)\epsilon} = \left(\delta p^{1-(n+1)\epsilon}\right) \cdot \frac{1}{\delta} \le \frac{1-(n+1)\epsilon}{1-n\epsilon}\,\delta^{\frac{1-n\epsilon}{1-(n+1)\epsilon}}\,p^{1-n\epsilon} + \frac{\epsilon}{1-n\epsilon}\left(\frac{1}{\delta}\right)^{\frac{1-n\epsilon}{\epsilon}}. \tag{3.6}$$

Then, estimating further (using $\delta^\lambda < \delta$),

$$c_0\,(\varphi, p^{1-(n+1)\epsilon}\varphi) \le c_0\,\delta\,(\varphi, p^{1-n\epsilon}\varphi) + c_0\,\frac{\epsilon}{1-n\epsilon}\,\delta^{-\frac{1-n\epsilon}{\epsilon}}\,(\varphi,\varphi). \tag{3.7}$$

With the choice $\delta := \min\{\frac{1}{2c_0}, \frac{1}{2}\}$, (3.3) is verified. □

Proof of Proposition.

We start by showing that $|(\varphi, V_k\varphi)| \le c\,(\varphi, p^{1-k\epsilon}\varphi)$ with some constant $c > 0$, such that the definition of μ_k in (ii) makes sense. Since $0 < (\varphi, p^{1-k\epsilon}\varphi) < \infty$ (for $\varphi \ne 0$), $\mu_k = 0$ implies $(\varphi, V_k\varphi) = 0$ which means that in this case V_k does not contribute to the expectation value of the transformed Dirac operator (2.9) and hence can be disregarded.
First we estimate the expectation value of V_1. According to (2.21), the symbol of V_1 is given by
$\hat{v}_1(\mathbf{q},\mathbf{p}) = \hat{v}(\mathbf{q}) - \hat{w}_1(\mathbf{q},\mathbf{p}) = -\frac{\gamma_0}{q^{2+\epsilon}}\,f_\epsilon\,(1 + \tilde{D}_0(\mathbf{q}+\mathbf{p}) \cdot \tilde{D}_0(\mathbf{p}))$. Since the multiplier of $q^{-(2+\epsilon)}$ is a bounded operator which is estimated by a constant, one finds according to (2.32) and (2.33) with $f(p) := p$

$$|(\varphi, V_1\,\varphi)| \le \frac{1}{(2\pi)^{3/2}} \int d\mathbf{p}\,|\hat{\varphi}(\mathbf{p})|^2\,I_1(p), \tag{3.8}$$

$$I_1(p) := \int d\mathbf{q}\; |\hat{v}_1(\mathbf{q}-\mathbf{p},\mathbf{p})| \left|\frac{f(p)}{f(q)}\right|^2 \;\leq\; c_1 \int d\mathbf{q}\; \frac{1}{|\mathbf{q}-\mathbf{p}|^{2+\epsilon}} \cdot \frac{p^2}{q^2}.$$

With the substitution $p\,\mathbf{q}' := (\mathbf{q}-\mathbf{p})$ one obtains for the latter integral

$$p^3 \int d\mathbf{q}'\; \frac{1}{(pq')^{2+\epsilon}}\; \frac{p^2}{|p\mathbf{q}'+\mathbf{p}|^2} \;=\; 2\pi\, p^{1-\epsilon} \int_0^\infty \frac{dq'}{q'^{1+\epsilon}}\; \ln\left|\frac{q'+1}{q'-1}\right| \;\leq\; c\cdot p^{1-\epsilon} \tag{3.9}$$

resulting in $|(\varphi, V_1\varphi)| \;\leq\; c_0\,(\varphi, p^{1-\epsilon}\varphi)$ where $c_1, c, c_0 \in \mathbb{R}_+$ are constants. Equation (3.4) completes the proof of (i) for $k = 1$. Note that since $\mu_1 = \inf c_0 > 0$, we have $|(\varphi, V_1\varphi)| > \frac{\mu_1}{2}\,(\varphi, p^{1-\epsilon}\varphi)$.

The proof of (ii) is by induction. First we show (ii) for $k=1$. From (2.12) we have $V_2 \;= i[V_1, B_1] \,+\, \frac{i}{2}\,[W_1, B_1] \,-\, W_2$ with W_2 from (2.37). Following the argumentation given in section 2.3 one can disregard the bounded operators $\tilde{D}_0$ in the estimates of p-form boundedness and consider V_2 as being represented by the commutator $[V, B_1]$.

With the modified Coulomb potential the symbol of B_1 which is proportional to $\hat{w}_1(\mathbf{q},\mathbf{p})$ according to (2.21), is estimated by $|\hat{\phi}_1(\mathbf{q},\mathbf{p})| \;\leq\; \frac{c}{q^{1+\epsilon}}\,\frac{1}{(q+p+1)^2}$.

The estimate of $|(\varphi, [V, B_1]\,\varphi)|$ is obtained from (2.46) by means of interchanging $\hat{\phi}_{n+1}$ with $\hat{\phi}_1$ and $|\mathbf{p}'{-}\mathbf{p}|^2$, $|\mathbf{p}'{-}\mathbf{q}|^2$ with $|\mathbf{p}'{-}\mathbf{p}|^{2+\epsilon}$, $|\mathbf{p}'{-}\mathbf{q}|^{2+\epsilon}$. Recalling that $|\hat{\phi}_1|$ can be replaced by its adjoint $|\hat{\phi}_1^*|$ and substituting $\mathbf{q}' := \mathbf{q}/p'$ in the first integral one obtains

$$|(\varphi, [V, B_1]\varphi)| \;\leq\; c \int d\mathbf{p}\; |\hat{\varphi}(\mathbf{p})|^2\; \{I_{11}(p) \;+\; I_{12}(p)\} \tag{3.10}$$

$$I_{11}(p) = \int d\mathbf{p}' \frac{1}{|\mathbf{p}'-\mathbf{p}|^{2+\epsilon}}\frac{p^2}{p'^2} \cdot \int d\mathbf{q}' \frac{1}{q'^2}\frac{1}{p'^{\epsilon}|\mathbf{q}'{-}\mathbf{e}_{p'}|^{1+\epsilon}(|\mathbf{q}'{-}\mathbf{e}_{p'}| + 1 + \frac{1}{p'})^2}$$

$$I_{12}(p) \;=\; \int d\mathbf{p}'\; \frac{1}{|\mathbf{p}'-\mathbf{p}|^{1+\epsilon}(|\mathbf{p}'-\mathbf{p}| \,+ p\,+1)^2}\; \frac{p^2}{p'^2} \cdot \int d\mathbf{q}\; \frac{1}{|\mathbf{p}'-\mathbf{q}|^{2+\epsilon}}\; \frac{p'^2}{q^2}.$$

For I_{11}, the $\mathbf{q}'$-integral is estimated by dropping $\frac{1}{p'}$ in the last factor of the denominator. Using (2.47) together with the substitution $\mathbf{k} := \mathbf{q}' - \mathbf{e}_{p'}$, one finds

$$\int \frac{d\mathbf{q}'}{q'^2}\frac{1}{|\mathbf{q}'-\mathbf{e}_{p'}|^{1+\epsilon}}\frac{1}{(|\mathbf{q}'-\mathbf{e}_{p'}|+1)^2} = \int_0^\infty dk \frac{k^{1-\epsilon}}{(k+1)^2}\cdot\frac{2\pi}{k}\ln\left|\frac{k+1}{k-1}\right| < \infty. \tag{3.11}$$

The $\mathbf{p}'$-integral results with the substitution $p\,\mathbf{p}'' := \mathbf{p}'$ and with the same techniques for the angular integration as applied in (2.34), in

$$\begin{aligned} p^2 \int d\mathbf{p}' \frac{1}{|\mathbf{p}'-\mathbf{p}|^{2+\epsilon}}\frac{1}{p'^{2+\epsilon}} &= p^{1-2\epsilon} \int_0^\infty dp'' \frac{1}{p''^{\epsilon}}\frac{2\pi}{\epsilon p''}\left(\frac{1}{|p''-1|^{\epsilon}} - \frac{1}{|p''+1|^{\epsilon}}\right) \\ &\leq\; c\cdot p^{1-2\epsilon} \end{aligned} \tag{3.12}$$

with a constant c.

I_{12} is treated in a similar way. The $\mathbf{q}$-integral is the one from (3.8) which is estimated by $c\,p'^{1-\epsilon}$. The remaining integral is estimated by replacing $|\mathbf{p}' - \mathbf{p}| + p + 1$ with $|\mathbf{p}' - \mathbf{p}| + p$. With the substitution $\mathbf{p}' =: p\mathbf{k} + \mathbf{p}$ and with the techniques from (2.34) one obtains

$$p^2 \int d\mathbf{p}' \, \frac{1}{|\mathbf{p}' - \mathbf{p}|^{1+\epsilon} \, (|\mathbf{p}' - \mathbf{p}| + p)^2 \, p'^{1+\epsilon}}$$

$$= p^{1-2\epsilon} \int_0^\infty \frac{k^{1-\epsilon} dk}{(k+1)^2} \cdot \frac{2\pi}{k(1-\epsilon)} \, \left[(k+1)^{1-\epsilon} - |k-1|^{1-\epsilon} \right] \le c \, p^{1-2\epsilon} \quad (3.13)$$

with some constant c. Using (3.7) and the definition of μ_k one thus obtains

$$|(\varphi, V_2 \varphi)| \le c_0 \, (\varphi, p^{1-2\epsilon} \varphi) \le c_0 \, \delta \, (\varphi, p^{1-\epsilon} \varphi) + C \, (\varphi, \varphi) \quad (3.14)$$

$$< \frac{2 c_0 \, \delta}{\mu_1} \, |(\varphi, V_1 \varphi)| + C(\varphi, \varphi)$$

with $2c_0\delta/\mu_1 < 1$ for a suitably chosen δ. This proves (ii) of Proposition 3.1 for $k = 1$.

The proof of the induction step from k to $k+1$ proceeds along the same lines as applied in section 2.3 to show the p-form boundedness of V_n and W_n. By induction hypothesis commutators of order $m \le k$ in the potential strength, denoted by $[\cdot]_m$, have the following symbol estimates (compare (2.43))

$$\int d\mathbf{q} \, \left(\left| \widehat{[\cdot]}_m (\mathbf{q} - \mathbf{p}, \mathbf{p}) \right| + \left| \widehat{[\cdot]}_m^{\,*} (\mathbf{q} - \mathbf{p}, \mathbf{p}) \right| \right) \left(\frac{p}{q} \right)^{2\lambda} \le c \, p^{1 - m\epsilon} \quad (3.15)$$

where λ can be chosen in the interval $]\frac{1}{2}, \frac{3}{2}[$. We demonstrate the proof for the commutator $[[\cdot]_m, B_{k-m+1}]$ which contributes to V_{k+1}. For the commutator $[V, B_k]$ which also contributes to V_{k+1} the proof is similar. Since the symbol classes of W_m and $[\cdot]_m$ are equal, it follows from (2.44)

$$|\hat{\phi}_m(\mathbf{q}, \mathbf{p})| \le \frac{c}{q + p + 1} \left| \widehat{[\cdot]}_m (\mathbf{q}, \mathbf{p}) \right| \le \frac{c}{q+1} \left| \widehat{[\cdot]}_m (\mathbf{q}, \mathbf{p}) \right|. \quad (3.16)$$

Then from (2.50), one has with some $c_0 \in \mathbb{R}_+$,

$$|(\varphi, [[\cdot]_m, B_{k-m+1}] \, \varphi)| \le \frac{c_0}{(2\pi)^3} \int d\mathbf{p} \, |\hat{\varphi}(\mathbf{p})|^2 \, (I_{00} + I_{01}) \quad (3.17)$$

$$I_{00} := \int d\mathbf{p}' |\widehat{[\cdot]}_m (\mathbf{p} - \mathbf{p}', \mathbf{p}')| \frac{p^2}{p'^2} \cdot \int d\mathbf{q} \frac{1}{|\mathbf{q} - \mathbf{p}'| + p' + 1} |\widehat{[\cdot]}_{k-m+1} (\mathbf{q} - \mathbf{p}', \mathbf{p}')| \frac{p'^2}{q^2}$$

$$I_{01} := \int d\mathbf{p}' \frac{1}{|\mathbf{p} - \mathbf{p}'| + p' + 1} |\widehat{[\cdot]}_{k-m+1} (\mathbf{p} - \mathbf{p}', \mathbf{p}')| \frac{p^2}{p'^2} \cdot \int d\mathbf{q} \, |\widehat{[\cdot]}_m (\mathbf{p}' - \mathbf{q}, \mathbf{q})| \frac{p'^2}{q^2}$$

where in the term denoted by I_{00}, $|\hat{\phi}_{k-m+1}(\mathbf{p}'-\mathbf{q},\mathbf{q})|$ was estimated by its adjoint before applying (3.16). In I_{01}, the $\mathbf{q}$-integral is by (3.15) estimated by $c\,p'^{\,1-m\epsilon}$. Further one has with $a \geq 0$ and $\delta > 0$

$$\int d\mathbf{q}\,\frac{1}{a+q+1}\,|\widehat{[\cdot]}_n(\mathbf{p}-\mathbf{q},\mathbf{q})|\,\frac{p^2}{q^2}\cdot q^{1-\delta} \;\leq\; p^{-\delta}\int d\mathbf{q}\,|\widehat{[\cdot]}_n(\mathbf{p}-\mathbf{q},\mathbf{q})|\,\frac{p^{2+\delta}}{q^{2+\delta}}$$

$$\leq\; c\,p^{1-n\epsilon-\delta} \tag{3.18}$$

if $1+\frac{\delta}{2}<\frac{3}{2}$. Then with $\delta := m\epsilon$, $\quad I_{01} \leq \tilde{c}\,p^{1-(k-m+1)\epsilon}\,p^{-m\epsilon} \;=\; \tilde{c}\,p^{1-(k+1)\epsilon}$. In I_{00} we estimate in the denominator $|\mathbf{q}-\mathbf{p}'|+p'+1$ by p' and subsequently use (3.15) to estimate the $\mathbf{q}$-integral by $c\,p'^{\,-(k-m+1)\epsilon}$. With $\lambda := 1+\frac{k-m+1}{2}\,\epsilon$ (for $(k-m+1)\epsilon<1$) in (3.15) we obtain $I_{00} \leq \tilde{c}\,p^{-(k-m+1)\epsilon}{\cdot}p^{1-m\epsilon} \;=\; \tilde{c}\,p^{1-(k+1)\epsilon}$. Therefore

$$|(\varphi,[[\cdot]_m,B_{k-m+1}]\,\varphi)| \;\leq\; c_0\,(\varphi,p^{1-(k+1)\epsilon}\varphi) \tag{3.19}$$

which proves (3.15) for $k+1$. The same estimate can be shown for $|(\varphi,[V,B_k]\,\varphi)|$. Hence

$$|(\varphi,V_{k+1}\varphi)| \;\leq\; c'\,(\varphi,p^{1-(k+1)\epsilon}\varphi) \;\leq c'\,\delta\,\frac{2}{\mu_k}\,|(\varphi,V_k\varphi)| \;+\; C\,(\varphi,\varphi) \tag{3.20}$$

which completes the proof of Proposition 3.1 (ii).
The proof of (i) for $k>1$ is again by induction. Assume V_k is p-form bounded with form bound $c_1<1$. Then we have from (ii)

$$|(\varphi,V_{k+1}\varphi)| \leq \delta|(\varphi,V_k\varphi)|+C(\varphi,\varphi) \leq \delta\,(c_1(\varphi,p\,\varphi)+C_1(\varphi,\varphi))+C(\varphi,\varphi). \tag{3.21}$$

Since δ can be chosen arbitrarily small, one has $\delta c_1<1$. A consequence of (3.21) is the p-form boundedness (with form bound <1) of every finite sum $V_1+...+V_n$.
For the proof of (iii) we have to show that all B_k are bounded operators. Then we can proceed as in section 2.4 to show that a unitary transform $U_k=e^{iB_k\tau}$ preserves the $p^{1-(n+1)\epsilon}$-form boundedness of the commutators of order $n+1$ in the potential strength of which $R^{(n+1)}$ is consisting. Consequently, one has with $(\varphi,p^{1-k\epsilon}\varphi)<\frac{2}{\mu_k}\,|(\varphi,V_k\varphi)|$ for $k=n+1$ and with (3.2),

$$|(\varphi,R^{(n+1)}\,\varphi)| \;\leq\; \text{const}{\cdot}|(\varphi,V_{n+1}\varphi)| \;\leq\; \text{const}{\cdot}\delta\;|(\varphi,V_n\varphi)|+C'\,(\varphi,\varphi) \tag{3.22}$$

with $\text{const}\cdot\delta<1$ for a suitably chosen δ. This shows the subordinacy with respect to V_n.
It remains to prove the boundedness of B_k. We will show this directly by using the algebra of symbol estimates. For B_1, from (2.57) with the substitution $\mathbf{q}' := \mathbf{q}-\mathbf{p}$,

$$I_{B_1} \;\leq\; \frac{c}{(2\pi)^{3/2}}\int d\mathbf{q}\,\frac{1}{|\mathbf{p}-\mathbf{q}|^{1+\epsilon}}\;\frac{1}{(|\mathbf{p}-\mathbf{q}|+q+1)^2}\cdot\frac{p^{1-\epsilon}}{q^{1-\epsilon}}$$

$$\leq \frac{c}{(2\pi)^{3/2}} \int d\mathbf{q}' \, \frac{1}{q'^{1+\epsilon}} \, \frac{1}{(q'+1)^2} \cdot \frac{p^{1-\epsilon}}{|\mathbf{p}+\mathbf{q}'|^{1-\epsilon}} \leq c' \tag{3.23}$$

since the integral is finite for $p \to 0$ and for $p \to \infty$ and the singularity of the last factor at $\mathbf{p} = -\mathbf{q}'$ is integrable. The convergence generating function $f(p) = p^{\frac{1-\epsilon}{2}}$ was chosen to allow for a (2.60)-type estimate when showing that the presence of U_k plays no role (but to prove boundedness of I_{B_1}, one can also take $f(p) = 1$).

For B_2, we use the estimate (2.44) of $\hat{\phi}_2$ by $\hat{w}_2$ and recall that W_2 is determined from the commutator $[V, B_1]$. Consider the symbol of VB_1 via (2.17),

$$|\widehat{v\phi_1}(\mathbf{q},\mathbf{p})| \leq \frac{c}{(2\pi)^{3/2}} \int d\mathbf{p}' \, \frac{1}{|\mathbf{q}-\mathbf{p}'|^{2+\epsilon}} \cdot \frac{1}{p'^{1+\epsilon}(p'+p+1)^2}. \tag{3.24}$$

It is found that $|\widehat{v\phi_1}(\mathbf{q},\mathbf{p})| = \text{const}$ for $p = 0$, $\sim 1/p^2$ for $p \to \infty$ and $\sim 1/q^{2+\epsilon}$ for $q \to \infty$ while it diverges for $q \to 0$. The behaviour near $q = 0$ is obtained by performing the angular integration with the help of a (2.34)-type formula such that one gets for $q \neq 0$, $\epsilon \neq 0$,

$$|\widehat{v\phi_1}(\mathbf{q},\mathbf{p})| \leq \frac{\tilde{c}}{q} \int_0^\infty \frac{dp'}{p'^\epsilon} \, \frac{1}{(p'+p+1)^2} \left(\frac{1}{|q-p'|^\epsilon} - \frac{1}{|q+p'|^\epsilon} \right). \tag{3.25}$$

Since the divergence at $q = 0$ results from the behaviour of the integral near $p' = 0$, it is sufficient to reduce the integration region to $[0,1]$ and estimate $(p'+p+1)^{-2} \leq 1$. The resulting integral can be performed analytically with the help of hypergeometric functions [7, p.284], and it behaves $\sim q^{1-2\epsilon}$ for $q \to 0$. B_1V is in the same operator class such that we obtain

$$|\hat{w}_2(\mathbf{q},\mathbf{p})| \leq c \, \frac{1+q^\epsilon}{q^{2\epsilon}(q+p+1)^2}. \tag{3.26}$$

By induction, one can show that for $k > 2$, one has $|\hat{w}_k(\mathbf{q},\mathbf{p})| \leq \frac{c}{(q+p+1)^{2+\epsilon}}$. Thus one obtains regularisation upon increasing k, resulting in bounded operators B_k, $k > 1$. $\square$

Proposition 3.1 provides justification for representing the transformed Dirac operator in terms of a series expansion in the potential strength. Note, however, that the limit $\epsilon \to 0$ cannot be carried out since in (3.7), $\frac{\epsilon}{1-n\epsilon}\,\delta^{-\frac{1-n\epsilon}{\epsilon}} \to \infty$ as $\epsilon \to 0$, which implies $C \to \infty$ in (3.3). Therefore, this limit cannot be used to prove for the Coulomb potential the p-form boundedness of V_k, $1 \leq k \leq n$ with form bound < 1. On the other hand, it has been shown with different tools that this property holds for V_1 and $V_1 + V_2$ in case of the Coulomb field [2, 8].

4 Proof of Theorem 1.2

The link between the two transformation schemes under consideration is provided by the following lemma.

Lemma 4.1. *Let* $H = D_0 + V$ *and* $U_j = e^{iB_j}$, $j = 1, ..., n$ *be the transformation scheme from section 2.1, where the potential term of k-th order in* γ *is decomposed into* $V_k + W_k$. *Let* U_0', $U_j' = e^{-iS_j}$, $j = 1, ..., n$ *be the Douglas-Kroll transformation scheme with the decomposition* $\mathcal{E}_k + \mathcal{O}_k$ *of the k-th order potential term. Then one has the identification*

$$\beta E_p = U_0' D_0 U_0^{'-1}, \qquad \mathcal{E}_k = U_0' V_k U_0^{'-1}, \qquad \mathcal{O}_k = U_0' W_k U_0^{'-1}$$

$$S_k = U_0' B_k U_0^{'-1}, \qquad k = 1, ..., n \tag{4.1}$$

with U_0' *from (1.5).*

The key observation is the relation between the spinor $\psi = \binom{u}{0}$ and the spinor φ in the positive spectral subspace of D_0,

$$\varphi = U_0^{'-1} \psi. \tag{4.2}$$

In momentum space, this equation is easily verified from $U_0^{'-1} = (\frac{\boldsymbol{\alpha}\mathbf{p}}{E_p+m}\beta + 1)\, A$ and from the explicit form (1.12) of $\hat{\varphi}(\mathbf{p})$. Then with the help of (2.6), the assertion (1.16) of Theorem 2.1 reads

$$\left(\varphi, (D_0 + \sum_{k=1}^{n} V_k)\, \varphi\right) = \left(U_0^{'-1} \psi, \sum_{k=0}^{n} H_k\, U_0^{'-1} \psi\right) = (\psi, H_n' \psi). \tag{4.3}$$

Identifying terms of fixed order $k \leq n$ and using (1.11), the assertion (4.3) is a consequence of

$$U_0' V_k U_0^{'-1} = \mathcal{E}_k, \qquad k = 1, 2... \quad \text{and} \quad U_0' D_0 U_0^{'-1} = \beta E_p \tag{4.4}$$

and hence of Lemma 4.1.

Proof of Lemma 4.1.

a) Verification of (4.1) up to first order in γ

The equality $U_0' D_0 U_0^{'-1} = \beta E_p$ is a consequence of (1.7) for zero potential. By means of explicit calculation (which for the sake of simplicity is only presented for the massless case $m = 0$), one gets from (2.18)

$$U_0' W_1 U_0^{'-1} = \frac{1}{\sqrt{2}} \left(1 + \beta \frac{\boldsymbol{\alpha}\mathbf{p}}{p}\right) \cdot \frac{1}{2} \left(V - \frac{\boldsymbol{\alpha}\mathbf{p}}{p} V \frac{\boldsymbol{\alpha}\mathbf{p}}{p}\right) \cdot \frac{1}{\sqrt{2}} \left(1 + \frac{\boldsymbol{\alpha}\mathbf{p}}{p} \beta\right)$$

$$= \frac{1}{2} \left[\beta \frac{\boldsymbol{\alpha}\mathbf{p}}{p} V - \beta V \frac{\boldsymbol{\alpha}\mathbf{p}}{p}\right] = \mathcal{O}_1 \tag{4.5}$$

and similarly, $U_0' V_1 U_0^{'-1} = \mathcal{E}_1$ with $V_1 = \frac{1}{2} \left(V + \frac{\boldsymbol{\alpha}\mathbf{p}}{p} V \frac{\boldsymbol{\alpha}\mathbf{p}}{p}\right)$. For the $m \neq 0$ case, one needs the relation $\frac{m}{E_p} + \frac{p^2}{E_p(E_p+m)} = 1$.

In order to prove $S_1 = U_0' B_1 U_0'^{-1}$ we first show that S_1 is uniquely determined by (1.10). Representing S_1 and $\mathcal{O}_1$ by their respective symbols s_1 and o_1 via (2.14) and noting that βE_p is a multiplication operator in Fourier space, one obtains from (1.10)

$$-\hat{o}_1(\mathbf{q},\mathbf{p}) \;=\; i\beta E_{|\mathbf{p}+\mathbf{q}|}\,\hat{s}_1(\mathbf{q},\mathbf{p}) \;-\; i\hat{s}_1(\mathbf{q},\mathbf{p})\,\beta E_p$$
$$= \; i\beta\left(E_{|\mathbf{p}+\mathbf{q}|} \;+\; E_p\right)\hat{s}_1(\mathbf{q},\mathbf{p}) \tag{4.6}$$

which can be uniquely solved for $\hat{s}_1(\mathbf{q},\mathbf{p})$. We now transform the defining equation (2.8) for B_1 with U_0'

$$U_0'\,W_1\,U_0'^{-1} \;=\; -i\,(U_0'D_0U_0'^{-1})(U_0'B_1U_0'^{-1}) \;+\; i\,(U_0'B_1U_0'^{-1})(U_0'D_0U_0'^{-1})$$
$$\Longleftrightarrow \qquad \mathcal{O}_1 \;=\; -i\,\left[\beta E_p, U_0'B_1\,U_0'^{-1}\right]. \tag{4.7}$$

From the uniqueness of the solution it follows from (4.7) and (1.10) that $U_0'B_1U_0'^{-1} = S_1$ and hence the uniqueness of the operator B_1.

b) Proof of (4.1) by induction for arbitrary order n in γ

We assume that to order $n-1$ the assertion of Lemma 4.1 holds. Then, the relation between the Dirac operators transformed to $n-1$st order, asserted by Theorem 1.2, is also true, i.e. (including the n-th order terms)

$$\beta E_p \;+\; \mathcal{E}_1 \;+\; \mathcal{E}_2 \;+ ... +\; \mathcal{E}_{n-1} \;+\; \mathcal{E}_n \;+\; \mathcal{O}_n$$
$$=\; U_0'\;(D_0 \;+\; V_1 \;+ ... +V_{n-1} \;+\; V_n \;+\; W_n)\;U_0'^{-1} \tag{4.8}$$

since $\mathcal{E}_n$ and $\mathcal{O}_n$ only depend on $\beta E_p,\ \mathcal{E}_j,\ \mathcal{O}_j,\ S_j,\ \ j=1,...,n-1,$ with the identical dependence of V_n and W_n on $D_0,\ V_j,\ W_j,\ B_j,\ \ j=1,...,n-1$. From (4.1) for $j=1,...,n-1$ it therefore follows that $\mathcal{E}_n = U_0'V_nU_0'^{-1}$ and $\mathcal{O}_n = U_0'W_nU_0'^{-1}$. Carrying out the n-th transformation one gets

$$U_n'\cdots U_0'HU_0'^{-1}\cdots U_n'^{-1} = \beta E_p + \mathcal{E}_1 + ... + \mathcal{E}_{n-1} + \mathcal{E}_n + \mathcal{O}_n + i[\beta E_p, S_n] + R_{n+1}$$
$$U_n^*\cdots U_1^*HU_1\cdots U_n = D_0 + V_1 + ... + V_{n-1} + V_n + W_n + i[D_0,B_n] + R^{(n+1)}. \tag{4.9}$$

B_n is obtained from $W_n = -i\,[D_0,B_n]$, or transformed with U_0',

$$U_0'\,W_n\,U_0'^{-1} \;=\; \mathcal{O}_n \;=\; -iU_0'\,[D_0,B_n]\,U_0'^{-1} \;=\; -i\,[\beta E_p, U_0'B_nU_0'^{-1}]. \tag{4.10}$$

Since the solution S_n to $\mathcal{O}_n = -i[\beta E_p, S_n]$ is unique, one gets $U_0'B_nU_0'^{-1} = S_n$. □

From the correspondence of the two transformation schemes it follows that for $n=2$, $H^{(2)}$ from (2.12) when acting on the positive spectral subspace of D_0, reduces to $\Lambda_+(D_0 + V + \frac{i}{2}\,[W_1,B_1])\Lambda_+$ since $i[V_1,B_1]$ corresponds to an odd operator which vanishes upon projection.

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